

**DEVELOPMENT OF LCSOFT AS A TOOL FOR LIFE CYCLE  
ASSESSMENT OF ENVIRONMENTAL IMPACTS: INCORPORATING  
ADDITIONAL LCIA METHODOLOGIES AND ENVIRONMENTAL  
FOOTPRINT**

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**Program:** Petroleum Technology

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Prof. Rafiqul Gani

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## ABSTRACT

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Tanathip Rattanatum: Development of LCSOFT as a Tool for Life Cycle Assessment of Environmental Impacts: Incorporating Additional LCIA Methodologies and Environmental Footprint

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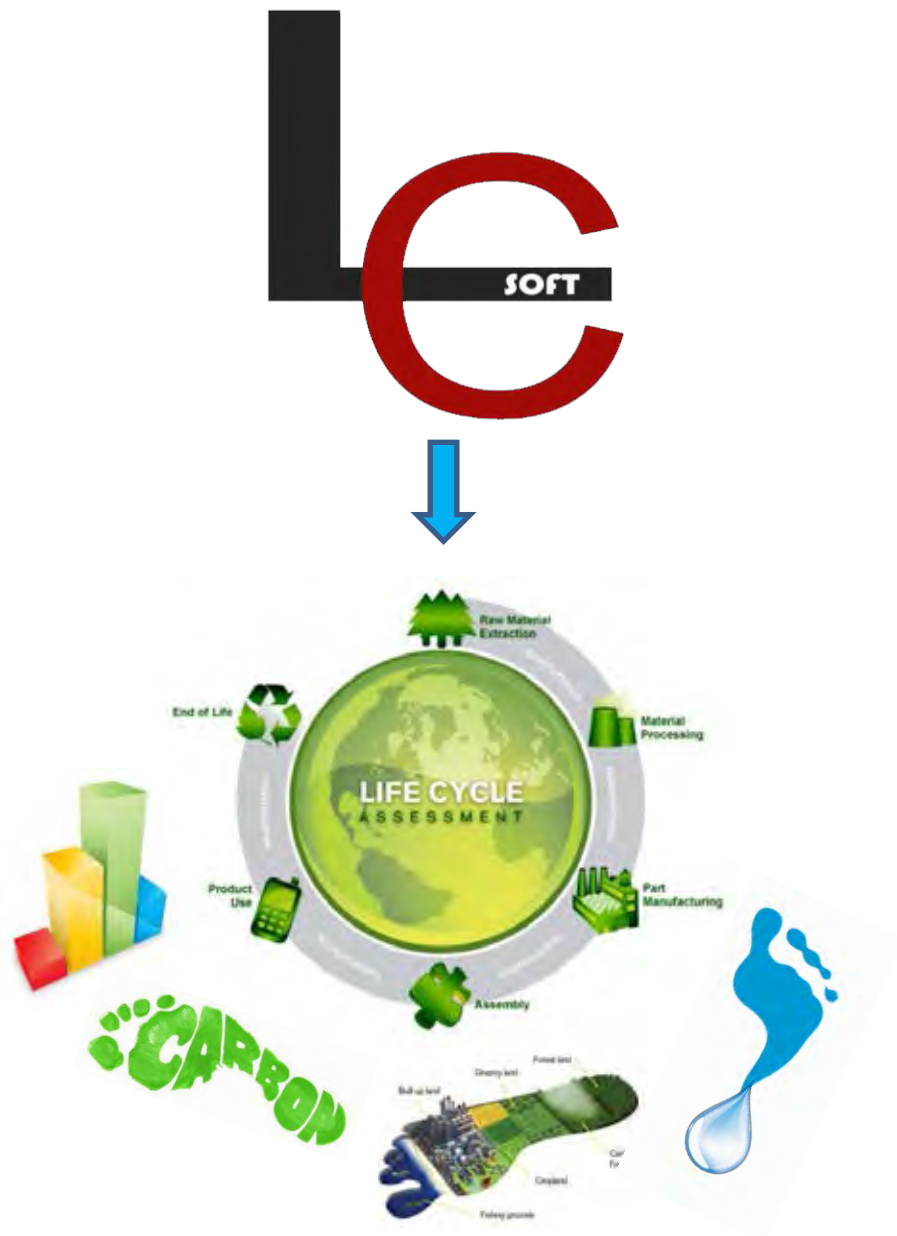
Life Cycle Assessment (LCA) is a technique to calculate, assess, and analyze environmental impacts through the entire life cycle of products. LCSOFT has been continuously developed as LCA software which has ability to integrate with other software e.g. process simulation software and economic analysis software. In addition, LCSOFT has several functions which can analyse various environmental effects such as sensitivity analysis, alternative comparison, and eco efficiency analysis. In this thesis, several features were added into LCSOFT to cover a wider application range from users and more industrial technologies. This thesis consists of four main parts. First, adding more essential equipment of industry and more operating conditions of column. Second, adding more LCIA methodologies to calculate environmental impacts of product. Third, including more impact assessment related to ecosystem by adding water scarcity footprint and ecological footprint. The last part is the validation of modification results by using two case studies: bioethanol from cassava rhizome and dimethyl carbonate from carbon dioxide capture and utilization process. By comparing with SimaPro v.8.3, the results calculated from LCSOFT show that the new version of LCSOFT has an ability to assess the environmental impacts precisely with the new features. Validation using two case studies proves that LCSOFT can be efficiently used to assess environment impacts from both biochemical and petrochemical processes.

## บทคัดย่อ

ธนาธิป รัตนารธรรม : การพัฒนาโปรแกรมแอลซีซอฟต์แวร์สำหรับการประเมินวัฏจักรชีวิตที่มีผลกระทบต่อสิ่งแวดล้อม: เพิ่มวิธีการประเมินผลกระทบทางสิ่งแวดล้อมใหม่และรอยเท้าสิ่งแวดล้อม (Development of LCSoft as a tool for Life Cycle Assessment of Environmental Impacts: Incorporating Additional LCIA Methodologies and Environmental Footprint) อ. ที่ปรึกษา : ผศ. ดร. ปมทอง มาลากุล ณ อยุธยา และ ศ. ดร. ราฟีก กานี 113 หน้า

การประเมินวัฏจักรชีวิตเป็นวิธีในการประเมินผลกระทบต่อสิ่งแวดล้อมตลอดช่วงชีวิตและต่อหน่วยของผลิตภัณฑ์ ซอฟต์แวร์แอลซีซอฟต์แวร์ได้รับการพัฒนาอย่างต่อเนื่องสำหรับการประเมินวัฏจักรชีวิตโดยมีความสามารถในการประยุกต์ใช้ร่วมกับซอฟต์แวร์อื่นเช่น ซอฟต์แวร์จำลองกระบวนการผลิตทางอุตสาหกรรมเคมี ซอฟต์แวร์ประเมินความคุ้มค่าทางเศรษฐศาสตร์ นอกจากนี้ซอฟต์แวร์แอลซีซอฟต์แวร์มีฟังก์ชันสำหรับนำเสนอผลกระทบต่อสิ่งแวดล้อมที่หลากหลายเช่น การวิเคราะห์ผลกระทบต่อข้อมูล การเปรียบเทียบกระบวนการและความคุ้มค่าทางเศรษฐศาสตร์ ในงานวิจัยนี้ซอฟต์แวร์ได้รับการเพิ่มเติมคุณสมบัติในหลายด้าน เพื่อรองรับการใช้งานที่หลากหลายจากผู้ใช้ ครอบคลุมเทคโนโลยีและวิธีการที่หลากหลายในอุตสาหกรรม โดยงานวิจัยนี้ได้แบ่งออกเป็นสี่ส่วนคือ ส่วนที่หนึ่งการเพิ่มอุปกรณ์ที่จำเป็นทางอุตสาหกรรมและเงื่อนไขในการดำเนินคอลัมน์กลั่นในอุตสาหกรรม ส่วนที่สองเพิ่มวิธีการเลือกในการคำนวณผลกระทบต่อสิ่งแวดล้อมของผลิตภัณฑ์ ส่วนที่สามเพิ่มการวิเคราะห์รอยเท้าสิ่งแวดล้อมนอกเหนือจากรอยเท้าคาร์บอนคือ รอยเท้าทางนิเวศน์และรอยเท้าของการขาดแคลนปริมาณน้ำซึ่งการวิเคราะห์ที่เพิ่มมานั้นล้วนเป็นสิ่งแวดล้อมทางธรรมชาติที่สำคัญ และส่วนที่สี่ตรวจสอบความถูกต้องของซอฟต์แวร์โดยการประเมินผลจากสองกรณีศึกษาคือกระบวนการผลิตไบโอเอทานอลจากเหง้ามันสำปะหลัง และการผลิตไบโเมทิลคาร์บอนเนตจากก๊าซคาร์บอนไดออกไซด์ผ่านกระบวนการจับก๊าซและนำไปใช้ประโยชน์โดยผ่านกระบวนการทางอุตสาหกรรม เมื่อทำการเปรียบเทียบผลกับซอฟต์แวร์การประเมินวัฏจักรชีวิตอื่น (ซิมาโปร v.8.3) ผลลัพธ์แสดงให้เห็นว่าซอฟต์แวร์แอลซีซอฟต์แวร์เวอร์ชันปัจจุบันมีความสามารถในการประเมินผลกระทบต่อสิ่งแวดล้อมได้อย่างแม่นยำ นอกจากนี้การวิเคราะห์ผลกระทบต่อสิ่งแวดล้อมผ่านสองกรณีดังกล่าวยังสามารถพิสูจน์ได้ว่าซอฟต์แวร์แอลซีซอฟต์แวร์สามารถวิเคราะห์ผลกระทบต่อสิ่งแวดล้อมได้ทั้งกระบวนการทางเคมีชีวภาพและกระบวนการทางปิโตรเคมี

# GRAPHICAL ABSTRACT



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## **CHAPTER I**

### **INTRODUCTION**

For decades, the growth of industries and increasing of population in the world are caused of more demand of source and more impacts to environment, such as climate change, eutrophication, resource depletion, and pollution in air, water and land. There are many policies in several countries to aware of those problem and claiming to be “green” or “sustainable”. Therefore, assessment of environmental has become the important key to improve and develop in many processes. One of the most popular techniques and widely used around the world is life cycle assessment, also known as LCA.

A Life cycle assessment or LCA is a popular tool for analysis and studying about environmental impacts of product. LCA is used for calculation and evaluation environmental impacts from inputs and outputs materials and energy of specific process. It quantifies every interrelated emission and resources consumption that emerged with all stages of product’s life and service system. LCA cover all stages of product’s life from raw materials acquisition through in every part of manufacturing process, transportation, used, disposal and recycling. The strength points of LCA are to identify and improvement the processes which are the problem in order to minimize environmental impacts and decrease using in natural source. Investigation all stages of product’s life there are huge and complicated data are required to calculate. At present, there are many commercial programs to study in LCA such as SimaPro, developed by Pre Consultants, Netherland, Gabi, developed by PE International, Deutshland, and etc. In the other views, there still need the software which includes the functions to others work such as integration with process design tools, economic analysis and sustainable development functions. Reason why our research group has created and developed the LCSofT software for assesses the effect from process, which product is interested, to environmental impacts.

A LCSofT is simple software in LCA and its feature has been design in the concept of user-friendly. LCSofT has been continuously developed by our research group from version 1.0 to 5.0 by Piyarak, 2012; Kalakul, 2013; Supawanich, 2014; Kaesinee, 2015 and Yodsathorn, 2016 respectively. LCSofT had ability to assess

environmental impacts, but there are opportunities to improve in performance and cover more application range of LCSOft.

Therefore, various aspects from previous mentioned will be improved in this research. Target in this project includes improvement and increase of new Life Cycle Impact Assessment (LCIA) methodologies and also new interpretations. In order to improve performances and extend application range and flexibilities of software, ReCiPe midpoint and endpoint impacts are added into LCIA method selection. Moreover, two new environmental footprints are added into interpretation including water scarcity footprint and ecological footprint. Finally, for more accuracy and comprehensive of LCSOft two case studies are validated environmental impact results with the commercial software, SimaPro version 8.3. Bioethanol from cassava rhizome process and dimethyl carbonate from carbon dioxide capture process are used as case studies in order to show that LCSOft has an ability to evaluate environmental impact from other kind of industrial processes, biochemical and petrochemical process. Not only environmental impacts result and carbon footprint of dimethyl carbonate produced from carbon dioxide capture and utilization process are calculated in this software, but water scarcity footprint and ecological footprint are also calculated by LCSOft.

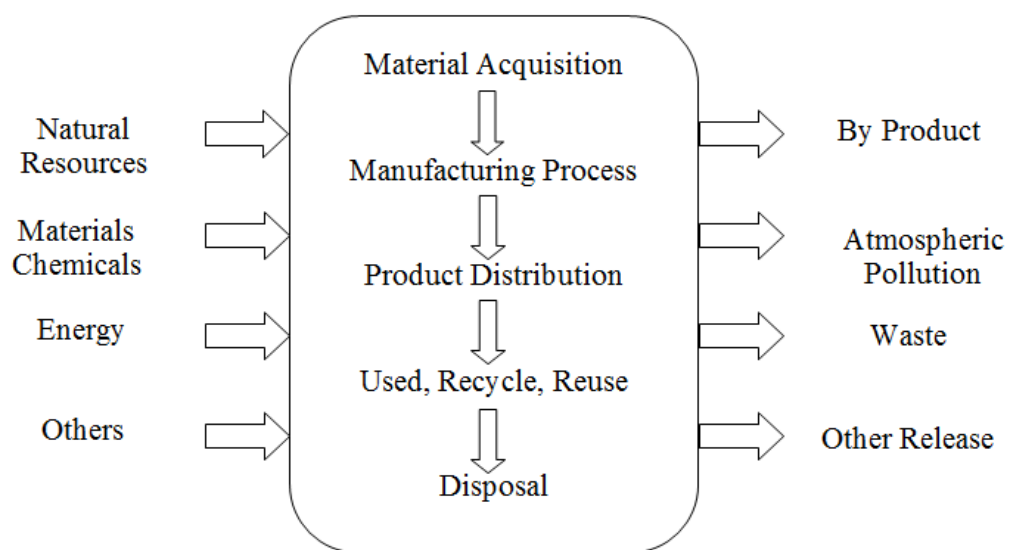
## CHAPTER II

### BACKGROUND AND LITERATURE REVIEW

This section consists of principle of Life Cycle Assessment (LCA) and development of LCSoft software. Description of LCA by following with principles, concepts and framework, first part, will help user understand the concept and results that reported by software. For second part will mention in development of LCSoft software from the first version to the latest version.

#### 2.1 Life Cycle Assessment (LCA)

Life Cycle Assessment is a systematic for calculation and evaluation environmental impacts from inputs and outputs materials and energy of specific process (Wikipedia, 2017b). It quantifies every interrelated emission and resources consumption that emerged with all stages of product's life and service system. LCA cover all stages of product's life from raw materials extraction through in every part of manufacturing process, transportation of raw material and product, used, disposal and recycling (Hoogervorst, 2004).

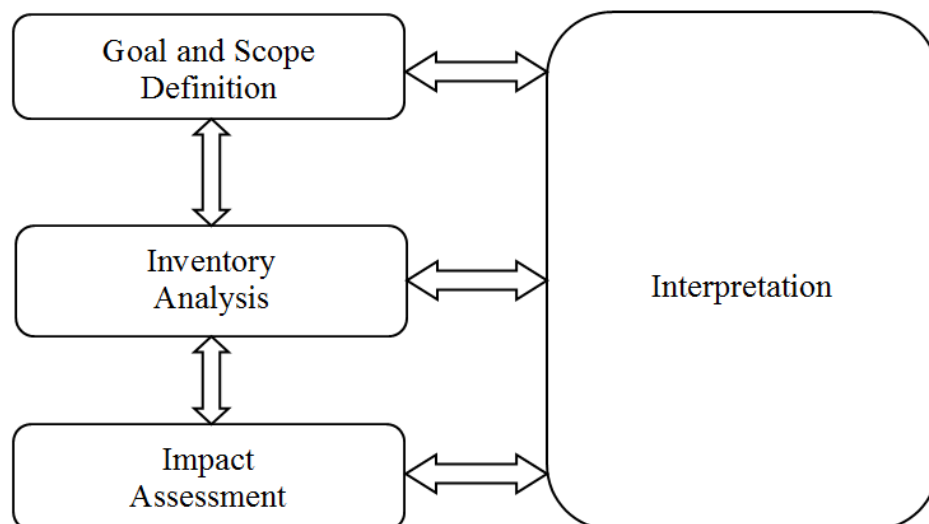


**Figure 2.1** All stages of product's life and input, output component (GDRC, 2017).



## 2.2 Steps of LCA

There are many worldwide organizations use an LCA to measure the environmental impacts from their product, reason why there are many different methods used by different users around the world. For advance and international standard of LCA, there are four main steps of LCA including goal and scope, life cycle inventory, life cycle impact assessment, and life cycle interpretation. The standard have been develop and all user knows as the International Organization for Standardization 14000 series (PRé, 2016).



**Figure 2.2** Four steps of LCA (Gjalt Huppés, 2006).

### 2.2.1 Goal and Scope

Life cycle of product or system life cycle is a common way of the complicated process, that mean the discrepancy in definition or data easily appear during the study. The easy and simple way to solve this problem is to define goal and scope in LCA study, which should be carefully illustrated former to initiation for inflows and outflows of the inventory. Normally, goal and scope should impose for carrying the LCA questions which answers is needed.

Goal of LCA can be different even though in same product or case study. Goal of study depend on the objective, such as to make comparison between

product or process, finding for some hotspot, providing data that use for internally or externally and decision making of user. Clearly description of this section is highly recommended in the first step of LCA study.

Scope of LCA that according with goal can be assigned by system boundaries, assumptions and limitations. Although initial set of data are added for iterative process in LCA. It can be adapted later if more information is available. There are four scopes of life cycle boundaries which users always consider.

#### *2.2.1.1 Cradle to Gate*

An evaluation which includes some part of product life cycle, carrying all material from natural source through the production, but excluding the end of life stages.

#### *2.2.1.2 Cradle to Grave*

This evaluation includes all parts of product life cycle carrying all materials from natural source through the end of life cycle stages.

#### *2.2.1.3 Gate to Gate*

An evaluation which is a partial speculates only value added to process in the production chain.

#### *2.2.1.4 Gate to Grave*

An evaluation which is a partial speculates from value added to process in the production chain to the end of life cycle stages (PRé, 2016).

### 2.2.2 Life Cycle Inventory (LCI)

LCI or Life Cycle Inventory is a very important step during LCA study because LCI is the straight-forward accounting of collection and calculation from plenty of data that gathered from several sources. All relevant data are collected such as, input, output, consumption of resource, waste flows, emissions, energy use, and others data from attributable from product's life cycle. Also, deeply details of all data, energy and raw materials, are tracked back to their original source and method or technologies that used to get that raw material and energy from source to enter and through the process until disposal. For example, electricity used in process can come from different source and production method, such as, coal, water, wind, nuclear and etc. Reason why, LCI analysis is extremely complex and can involve several of

specific or individual unit processes in supply chain, extraction of raw resource, various of primary and secondary production processes, differently of transportation, etc. LCI data will be used to estimate for the environmental impact latter.

Although a lot of data is available in various places, missing of data collection usually encounter while studying of LCA. However there are techniques for more correct missing data. For collecting data, foreground and background are used to distinguish between different types of data.

Foreground data is collected from particular process directly. Various ways to gather particular process data are questionnaire, interviews, or stream table from specific source.

Background data is the generic data, such as, materials, transportation, energy consumption, and waste. This data are always available in public and commercial database or in literatures, which do not need to make a questionnaire or others ways to collect data same as foreground data. However, there are some available database and limited access database of LCI. Table 2.1 and 2.2 are shown the online LCI databases from different regions in the world.

**Table 2.1** Available life cycle inventory databases, number of datasets (Curran, 2006b)

Name	Website	Availability	Language	Date Focus (if any)	Number of Datasets	Geographic Origin
Australian Life Cycle Inventory Data Project	<a href="http://www.auslci.com.au/">http://www.auslci.com.au/</a>	Free	English		100	Australia
BUWAL250	<a href="http://svi-Verpackung.ch/de/Services/1&amp;Publikationen/">http://svi-Verpackung.ch/de/Services/1&amp;Publikationen /</a>	Fee or included with SimaPro	German, French	Packaging materials		Switzerland
Canadian Raw Material Database	<a href="http://crmd.uwaterloo.ca/">http://crmd.uwaterloo.ca/</a>	Free with registration	English, French	Aluminum, glass, plastics, steel, and wood	17	Canada
ecoinvent	<a href="http://www.ecoinvent.ch">www.ecoinvent.ch</a>	License fee	English		4000	Global/Europe/Switzerland
EDIP	<a href="http://www.lca-center.dk">www.lca-center.dk</a>	License fee	Danish		100	Denmark

**Table 2.1** Available life cycle inventory databases, datasets (cont.) (Curran, 2006b)

Name	Website	Availability	Language	Date Focus (if any)	Number of Datasets	Geographic Origin
German Network on Life Cycle Inventory Data	<a href="http://www.lci-network.de">www.lci-network.de</a>	On-going	German, English			Germany
LCA Food	<a href="http://www.lcafood.dk">www.lcafood.dk</a>	Free	Danish, English	Food products and processes		Denmark
SPINE@CPM	<a href="http://cpmdatabase.cpm.chalmers.se/">http://cpmdatabase.cpm.chalmers.se/</a>	Free	English		700	Global
Swiss Agricultural Life Cycle Assessment Database (SALCA)	<a href="http://www.agroscope.admin.ch/oekobilanzen/">http://www.agroscope.admin.ch/oekobilanzen/</a>	Available throughecoinvent or with project cooperation	German, English, French, Italian	Agriculture	700	Switzerland
Thai National LCI Database	<a href="http://www.thailcidatabase.net">http://www.thailcidatabase.net</a>		Thai, English			Thailand
US LCI Database Project	<a href="http://www.nrel.gov/lci">www.nrel.gov/lci</a>	Free with contact	English		300	USA

**Table 2.2** Available life cycle inventory databases, product group (Curran, 2006b)

Industry Organization	Website	Availability	Language	Product Group or Sector	Geographic Coverage
American Plastics Council (APC)	Available from US LCI	Free	English	Polymers	America
EPD-Norway	<a href="http://www.epd-norge.no">www.epd-norge.no</a>	Free	Norwegian, English	Norwegian business (several sectors)	Norway and Europe
European Aluminium Association (EAA)	<a href="http://www.aluminium.org">www.aluminium.org</a>	Free	English	Aluminium production	Europe
European Copper Institute (ECI)	<a href="http://www.copper-life-cycle.org">www.copper-life-cycle.org</a>	Free with contact	English	Copper tubes, sheets and wire	Europe
European Federation of Corrugated Board Manufacturers (FEFCO)	<a href="http://www.fefco.org">www.fefco.org</a>	Free	English	Corrugated Board	Europe

**Table 2.2** Available life cycle inventory databases, product group (cont.) (Curran, 2006b)

Industry Organization	Website	Availability	Language	Product Group or Sector	Geographic Coverage
International Iron and Steel Institute (IISI)	<a href="http://www.worldsteel.org">www.worldsteel.org</a>	Free with contact	English	Steel	Global
International Zinc Association	<a href="mailto:info@iza.com">info@iza.com</a>	Available to LCA practitioners on request	English	Zinc	Global
ISSF International Stainless steel Forum (ISSF)	<a href="http://www.worldstainless.org/">www.worldstainless.org/</a>	Free with contact	English, Chinese, Japanese	Stainless steel	Global
KCL (EcoData)	<a href="http://www.kcl.fi/">http://www.kcl.fi/</a>	Free	English	Pulp and paper	Finish/Nordic
Nickel Institute	<a href="http://www.nickelinstitute.org">http://www.nickelinstitute.org</a>	Free with contact	English	Nickel	Global
Volvo EPDs	<a href="http://www.volvotruck.com/dealers-utc/en-gb/VTBC-EastAnglia/aboutus/environment/environmental_product_declaration">http://www.volvotruck.com/dealers-utc/en-gb/VTBC-EastAnglia/aboutus/environment/environmental_product_declaration</a>	Free	English	Trucks and busses	Europe
World Steel Carbon Footprint	<a href="http://www.worldautosteel.org/Environment/Life-Cycle-Assessment/worldsteel-releases-datasets-to-help-lower-carbon-footprint.aspx">http://www.worldautosteel.org/Environment/Life-Cycle-Assessment/worldsteel-releases-datasets-to-help-lower-carbon-footprint.aspx</a>	Free by request	English	Steep Products	Global

### 2.2.2.1 Matrix calculation in Life Cycle Inventory

In LCSOFT, matrix calculation is used in Life Cycle Inventory (LCI) phase. This method was represented by (Heijungs & Suh, 2002). There are two main matrix equations as shown in the following equations for calculate LCI result.

$$As = f \quad (1)$$

A is the abbreviation of “Technology Matrix”

s is the abbreviation of “Scaling Factors”

f is the abbreviation of “Final Demand Vector”

$$g = Bs \quad (2)$$

g is the abbreviation of “Total Intervention Matrix”

B is the abbreviation of “Intervention Matrix”

s is the abbreviation of “Scaling Factors”

#### 2.2.2.2 Allocation

Normally in LCI calculation phase, there are collected inventory data of interesting product which identify the input and output data from process. Although product that user interests will report the result after calculation there are other process that can produce more than one product per raw material, *multifunctional process*. For example, Crude oil in refinery is fed in to process and several of products are produced, jet fuel, diesel, gasoline and etc. Therefore, in the case of production process with more than one product, an allocation is applied for dividing the environmental loading. The emissions from process are separated into each product and co-product. There are two types of allocation, physical allocation and economic allocation. Physical allocation is the facility that used in process and total resource consumption and for economic allocation may be considered as a representative for market based (BV, 2015).

#### 2.2.3 Life Cycle Impact Assessment (LCIA)

All data that collected from previous steps, Goal and Scope and LCI, will be analyzed into differently environmental impact by calculation in LCIA section. This step is the process to calculate the environmental impacts which occur from products or processes and make results to the data which easy for audience to understand. Plenty of substances degraded to the environment, with each substance are causes of different midpoint environmental impact categories, such as, acidification, climate change, eutrophication, stratospheric ozone depletion, human toxicity and depletion of resource. Each midpoint impact categories can combine together into endpoint environmental impact categories that effect from associated midpoint, human health, natural environmental and natural resource. There are many of LCIA methodologies that consists of different in number of midpoint and endpoint impact categories also characterization and normalization factors in each component. For international standard of assessment method ISO coming to defines the distinction between imperative elements and optional elements.

### *2.2.3.1 Imperative Elements*

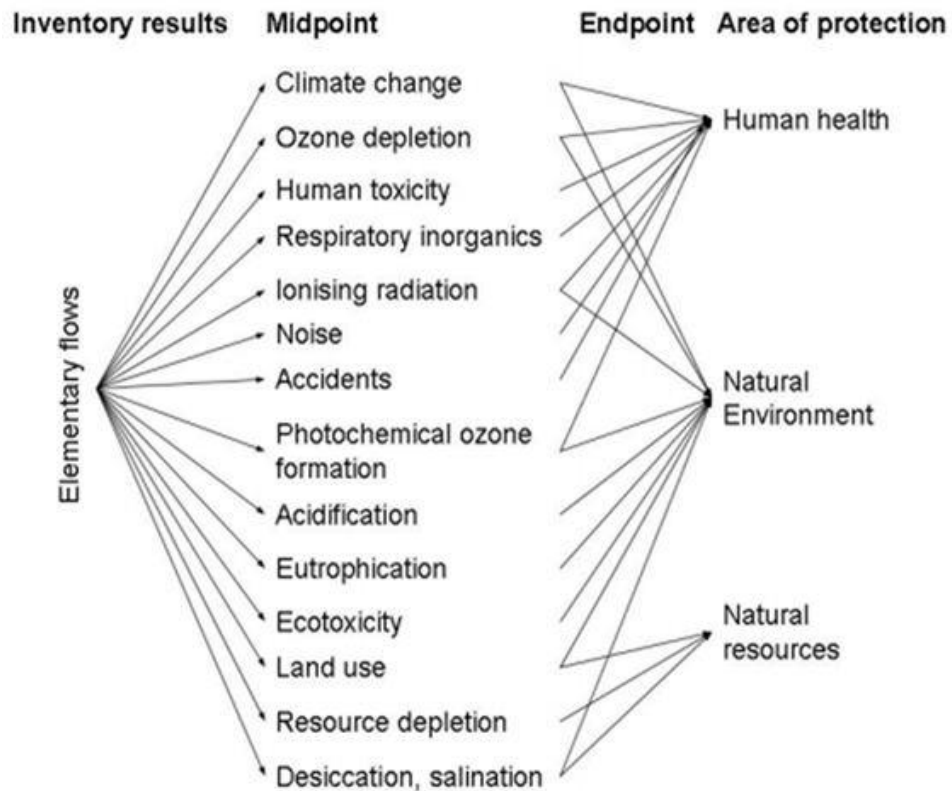
Imperative elements are the method which users have to do during the LCIA step concluding with selection and definition of impact categories, classification and characterization.

#### *2.2.3.1.1 Selection and Definition of Impact Categories*

Selection and definition of impact categories is the first important step in an LCIA. There are two levels of impact, Midpoint and Endpoint level.

Midpoint level of impact categories demonstrate the influence of the release substance somewhere along the process, but before the end of the process (ILCD, 2010a). Results in this level always focus in a point of environmental impact and depend on several of substances that effect to the specific impact categories, such as Acidification, Ozone depletion, Eutrophication, Ecotoxicity, Resource depletion and etc. (Curran, 2006a).

Endpoint level of impact categories demonstrate the effect at the end of the process by formulate many data from midpoint level. Data from midpoint are combined to one endpoint impact category also known as three Areas of Protection which includes Human health, Ecosystem quality and Natural resource. However, endpoint is optional function in LCA study and there is high uncertainty from data gap and more assumption along the process.



**Figure 2.3** Midpoint and Endpoint impact categories (ILCD, 2010a).

Even though there are advantages and disadvantages in midpoint and endpoint level of impact categories, the selection of any LCIA method should meet the requirement of the national standard and according to the goal and scope of LCA which is considered in each study (ILCD, 2010a; Rebitzer et al., 2004).

#### 2.2.3.1.2 Classification

The second assigning of the elementary flows for impact assessment at all level, midpoint and endpoint, is to assign one or more interrelated impact categories or selected impact categories. For example, carbon dioxide (CO<sub>2</sub>) emission will be classified into category of climate change. For other elements are not exclusive to one impact category, so they can be classified in two or more impact categories, such as, sulfur dioxide (SO<sub>2</sub>) is needed to distinction



between two impact categories, human health and acidification which both of them are parallel mechanisms (ISO 14044, 2008; ILCD, 2010b).

### 2.2.3.1.3 Characterization

Last imperative step of LCIA step is characterization. To compare different inventory data, input and output data, science based conversion factors, this factors is called characterization factors, are used. Characterization used to convert LCI results into representative indicators for each impact categories. However, there is simple calculation by using the following equation:

$$\text{Inventory Data} \times \text{Characterization Factor} = \text{Impact Indicators} \quad (3)$$

Characterization can convert different quantities of chemical into an equal magnitude to measure the amount of impact on each impact categories (GmbH, 2017). For each method there is different in quantity in midpoint and endpoint impact categories as shown in Table 2.3.

**Table 2.3** Midpoint and Endpoint in each method (Gjalt Huppel, 2006)

Distance-to-Target	Midpoint	Endpoint
Critical Volumina	CML (9+)	EPS (5)
Ecological Scarcity	EDIP (9)	Eco-indicator 99 (3)
	TRACI (12)	
	ILCD Handbook (15)	ILCD Handbook (3)
	<b>Midpoint-Endpoint</b>	
	IMPACT 2002+ (14-4)	
	LIME (11-4)	
	ReCiPe (18-3)	
	IMPACT World+ (30-3)	

The International Reference Life Cycle Data System was developed by the Institute for Environment and Sustainability in the European Commission Joint Research Centre (JRC) is based on ISO 14040/44 standard. ILCD handbook is guidance for assessing the emissions and consumption of resource in

term of environmental impacts with suitable methodology. For ILCD methodology, there are fifteen midpoint impact categories.

Acidification caused by the emissions of airborne and/or acidifying chemicals from process. That increases the concentration of hydrogen ion in water and soil. Ammonia (NH<sub>3</sub>), nitrogen oxides (NO<sub>x</sub>) and sulphur dioxide (SO<sub>2</sub>) are the main substances that are released from process and caused of acidification (ILCD, 2010a, 2010b).

Climate change use Global Warming Potential to evaluate the irradiative forcing over period years, such as 20, 100 or 500 years, or residence time of substance, developed by the Intergovernmental Panel on Climate Change (IPCC) (ILCD, 2010a, 2010b).

Terrestrial eutrophication is the excessive of nutrient salt concentration in terrestrial environmental. That cause by the emissions from several substances, such as nitrogen and ammonia (Rosenbaum, 2009).

Marine eutrophication can be described with the enrichment of the nutrient in sea or ocean environmental. Water quality will decrease because plankton, algae and sea plants (Rosenbaum, 2009).

Freshwater eutrophication can be described with the enrichment of the nutrient in lake, river or water environmental. Water quality will decrease because blooming of plankton, algae and aquatic plants (Rosenbaum, 2009).

Freshwater ecotoxicity: Freshwater is the most important factor for human life. This part will evaluate and compare the toxic for freshwater of ecosystem.

Human toxicity – carcinogenics: Evaluating the effects of toxicological that cause of abnormality on human health and cancer disease (Rosenbaum, 2009).

Human toxicity - non-carcinogenics: Evaluating the effects of toxicological that cause of abnormality on human health.

Ionizing radiation – human health calculate amount of radionuclides that can be exposed to environmental and caused to human directly (Zoran Steinmann, 2015).

Land use consider the main threats that occur with soil and its properties, such as erosion, loss of biodiversity, sealing, compaction, salinization and decreasing of soil organic matter (SOM) (Vidal Legaz et al., 2017).

Particulate matter/respiratory inorganics are a caused of health problems. Fine particulate matter is represent as a mixture of inorganic and organic substances (Mark Goedkoop et al., 2009).

Ozone depletion occurs because emissions of ozone depleting substances (ODS). These substances contain with chlorine or bromine atoms. Ozone depletion capacity that occurs with ODS is defined by Ozone Depletion Potential (ODP) (Mark Goedkoop et al., 2009).

Photochemical ozone formation generated pollutants by changing the reactive nature with oxidizing organic molecules on surfaces. The impact pathway is very complex and depend on the concentration of VOC (ILCD, 2010a, 2010b).

Resource depletion – mineral, fossils and renewables: are naturally occurring substances in natural processes. More decreasing availability of total reserve comparing with their replacement rate is definition of resource depletion in that sources (Rosenbaum, 2009).

Resource depletion – water: Decreasing of fresh water in natural source is the essential topic to consider and there are many policies to adjust amount of water used (Mark Goedkoop et al., 2009).

**Table 2.4** Midpoint impact categories reference unit (Sébastien Humbert, 2012)

<b>Impact Categories</b>	<b>Reference Unit</b>
Acidification	Mole H <sup>+</sup> eq.
Climate change	kg CO <sub>2</sub> eq.
Terrestrial eutrophication	Mole N eq.
Marine eutrophication	kg N eq.
Freshwater eutrophication	kg P eq.
Freshwater ecotoxicity	CTUe
Human toxicity - carcinogenics	CTUh
Human toxicity - non-carcinogenics	CTUh
Ionizing radiation - human health	kg U <sub>235</sub> eq.
Land use	kg SOC
Particulate matter/Respiratory inorganics	kg PM <sub>2.5</sub> eq.
Ozone depletion	kg CFC-11 eq.
Photochemical ozone formation	kg C <sub>2</sub> H <sub>4</sub> eq.
Resource depletion - mineral, fossil and renewable	kg Sb eq.
Resource depletion - water	m <sup>3</sup>

### 2.2.3.2 *Optional Elements*

Optional elements, normalization, grouping, sensitivity and uncertainty analysis, are the functional step for users to select the following step in calculation or not.

#### 2.2.3.2.1 *Normalization*

Normalization is used to simplify the results, which relative to the reference values, in interpretation step. Results which have different units are converted into dimensionless quantities by multiply results of impact assessment with normalization factors for facilitate in comparison between distinguish impact categories (Rebitzer et al., 2004). Normalization result which unit is dimensionless unit, will be compared with the reference value (normal value) and the results will show higher or lower from reference value that are relate to a community, person or others system.

Normalization factors for each impact category and country are obtained by multiplying with characterization factors respectively with their emission. Summation in every impact category is the normalization factor (Rosenbaum, 2009).

#### *2.2.3.2.2 Grouping*

User can reduce confusion from several impact categories by minimizing number of impact categories. Indicators from different impact categories are combined into a set and ranked the important of that category.

#### *2.2.3.2.3 Weighting*

Multiplying score of each impact categories by the weighting factor for adjust the result from impact that reflects to the goal of study.

### 2.2.4 Interpretation

Interpretation is the last step of LCA. Data from LCI, LCIA and previous step are considered together. In this step, the results and conclusions are derived from the assessment, which report is easy to understand, transparent manner and consistent with goal and scope (ISO 14040, 2008; ILCD, 2010b).

#### *2.2.4.1 Contribution Analysis*

This is an important step to understand the results from LCI and LCIA calculation. The results show the relative contribution of product's life and the important roles that caused of environmental impacts, which help the user see the exactly problem of process in LCA (PRé, 2016).

#### *2.2.4.2 Sensitivity Analysis*

Sensitivity analysis is recalculated for the influence when there are something change, such as important assumption, system boundary, amount of utility and characterization (PRé, 2016).

#### *2.2.4.3 Uncertainty Analysis*

Data are input into LCA for calculate environmental impact. The data are collected from several sources and different reliability, for example different in location, time, community and purpose. Therefore, uncertainty analysis considers the influence that effect from previous reasons. The results after uncertainty analysis are shown in range, percentage of result or the different from the

true value, which already includes uncertainty values. Input data are calculated with a probability distribution and stores the output data from calculation. There are repeated several times to be sure that input value represent the effect from the selected distribution. Calculation with the uncertainty analysis can be expressed by eq. (4) (Zoran Steinmann, 2015).

$$f(x) = f(x_t + \Delta x) = y_t + \Delta y = y \quad (4)$$

$\Delta x$  is the error in  $x$

$x$  is the observed or measured value for  $x$  variable

$x_t$  is the true value for  $x$

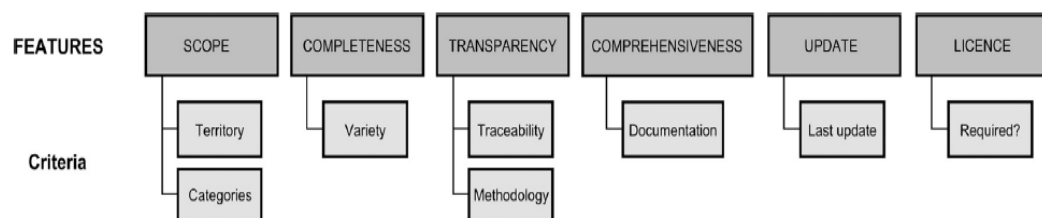
$\Delta y$  is the error in  $y$

$y$  is the observed or measured value for  $y$  variable

$y_t$  is the true value for  $y$

### 2.3 Main Features of LCA Databases

Several of databases are used for the study of environmental impact, however there are several problems to select the proper database for each case such as the location of database and process, which is evaluated, do not match, obscure of transparency or unsuitability. In this situation, LCA is the most popular tool for evaluate the sustainability or unsustainability in every industry reason why following features which are shown in Figure 2.4 will help users make a better selection for LCA databases (Martínez-Rocamora et al., 2016).



**Figure 2.4** Feature and criteria for the evaluation of LCA databases (Martínez-Rocamora et al., 2016).

For comparison among various LCA databases, the following feature lists are proposed.

#### 2.3.1 Scope

There are two criteria for scope of LCA database. The first is territory between database and location that case study take place.

#### 2.3.2 Completeness

The main criterion of completeness is how the database can cover all of existent of materials and categories which are considered.

#### 2.3.3 Transparency

The traceability and the obviously of the methodological processes line which the life cycle of the materials are evaluated (LCI and flow diagrams) which is the core in LCA.

#### 2.3.4 Comprehensiveness

Plenty of information is provided for LCA consideration, the integrity of documentation is importance because it is a necessary factor to adapt or make modifications to another study.

#### 2.3.5 Update

Approximate of the latest update of database and project under evaluation is important for accuracy results.

#### 2.3.6 License

Many databases are license database, user has to pay for access and there are some free databases which user can access without pay.

Results from using six features and criteria to compare among different databases are shown in Table 2.5 which the results are score by + and – signs (+: partially or accomplished sometimes, -: not accomplished).

**Table 2.5** Comparison of LCA database (Martínez-Rocamora et al., 2016)

FEATURE	Criterion	Ecoinvent	ELCD	GaBi	PlasticsEurope	Athena	U.S.LCI	Base Carbone
SCOPE	Territory	+++	+++	+++	+++	++	+	+
	Categories	+++	++	+++	+	+++	+++	+++
COMPLETENESS	Variety	+++	++	+++	+++	++	++	++
TRANSPARENCY	Traceability	+++	+++	+++	+++	NA.	+	+++
	Methodology	+++	+++	+++	+++	NA.	++	+
COMPREHENSIVENESS	Documentation	+++	+++	+++	+++	NA.	+	+
UPDATE	Last update	2012	2012	2012	2012	2012	2012	2013
LICENCE	Required	Yes	No	Yes	No	Yes	No	No

## 2.4 Environmental Indicators

Over the past couple of decades, new trend of industrial more consider in environmental impacts, which are the effects from their process reason why LCA is used to evaluate in the different environmental impacts. For easier to communication and understanding by the audience, indicators in some environmental impacts are created.

### 2.4.1 Carbon Footprint

LCA represents the indicator, which use for measure the impact from human activities by quantifying the amount of carbon dioxide emission and other greenhouse gases (GHG) in term of carbon dioxide equivalent (CO<sub>2</sub>e), also known as carbon footprint. Carbon dioxide equivalent will be converted into global warming potential (GWP) by multiplying the emissions of each GHG. Carbon footprint is easier to communicate and understand by audiences than full LCA report, which is the one advantage of carbon footprint (Thøgersen & Nielsen, 2016).

Global Warming Potential (GWP) is the quantity of amount of heat or greenhouse gas trap in the atmosphere. Unit of GWP is over a specific time interval, 20, 50, 100 or 500 years (Kaldellis & Apostolou, 2017). GWP is represented the same amount of CO<sub>2</sub>. There are emissions factor (EF) to convert the amount of others elements into CO<sub>2</sub>e for comparing the GHG effects in same unit (CO<sub>2</sub>e) and evaluate amount of GWP (Wikipedia, 2017a).

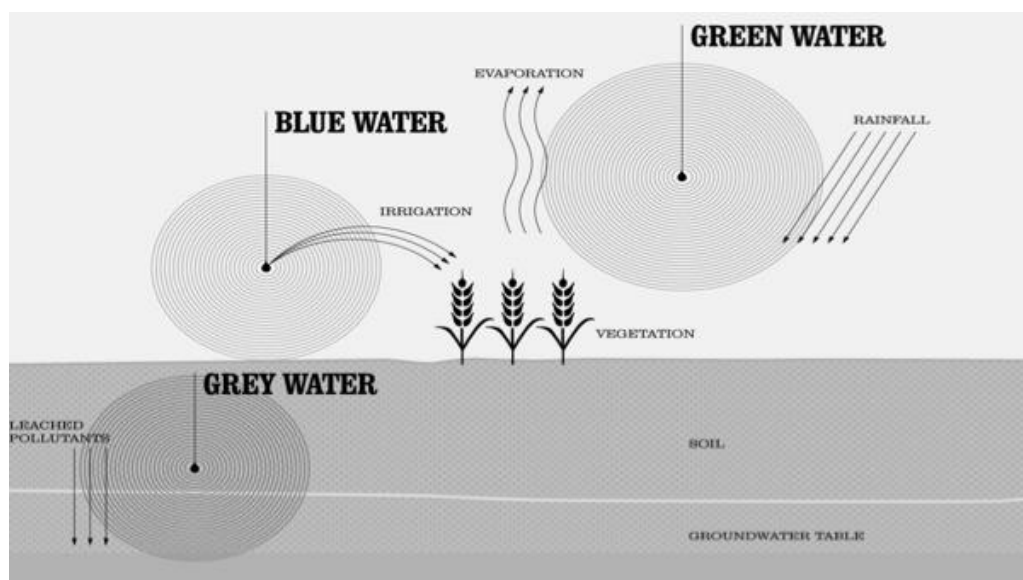


### 2.4.2 Water Scarcity Footprint

Water is the most important natural resource. All human activities always consume water, which is the main key component in each activity. Rapidly growth of industry and population increasing are the cause of growing in demand of resource, including water, and quality change. One technique to solve this situation is water footprint based on LCA. For international standard, ISO 14046 is published for the standard of assessing and reporting result of water footprint (Footprint, 2017).

ISO 14046 is the international standard which is specify for the principles, guidelines and requirements of evaluating and reporting water footprint based on LCA (BSIGROUP, 2017).

The water footprint measures the amount of water used by human activities, volume of water consumed, and polluted. Water footprint report depend on the goal and scope or questions from user. It can be measured and assessed in several units, such as cubic metres per tonne, per acre of cropland, per unit, per tonne of production and etc. There are three components of water, green, blue and grey. Each type of water is specified by the different source of water consumed, which is showed in Figure 2.5.



**Figure 2.5** Components of water footprint (Footprint, 2017).

Green water footprint is used to measure amount of rainwater used during the process particularly interrelate with agricultural, products, based on crop or wood, and water used during the harvest. Green water is water from the precipitation on land and does not implicate with groundwater, but this water is kept in the soil or temporarily on top of surface or vegetation. Finally, this precipitation evaporates or migrates through plants (WaterFootprint, 2017c).

Blue water footprint is used to measures the volume of water on surface and ground water used for the production. Definition of blue water used is the volume of freshwater consumed, evaporated or incorporated to product and includes water from surface and ground water in a reservoir that returned to another reservoir or the sea. Agriculture, domestic and industry always use blue water (WaterFootprint, 2017a).

Grey water footprint is the freshwater that associated for adjust the pollutants to meet the standard quality. Grey water footprint calculates the volume of freshwater that is used to dilute pollutants in production phase based on natural background, concentrations and water quality standard. Eventually, after treating the quality of water and concentration of pollutants have to meet the quality standard (WaterFootprint, 2017b).

Normally in LCA calculation only amount of blue and grey water are calculated in water footprint. There are many methods published for calculate water footprint, but scarcity of water in different country, which is an important factor, is not included during the calculation that will make some errors from inequality of water available in each country. Water Use in Life Cycle Assessment (WULCA) group use more than eight years to create new methodology which based on the quantity of the available water per area of interest country. This calculation of water scarcity footprint is also corresponding to the ISO standard. The ranges of characterization factor (CF) are 0.1 to 100. (Boulay et al., 2017).

Characterization factors have been developed in the past decade. WTA or water withdrawal-to-availability were used as a characterization factors, but WTA does not correspond to ISO 14046 in the aspects of water quality. Hence, consumption-to-availability or CTA ratio were developed to be a characterization factor, however, this characterization does not contribute to water scarcity in each

country. From WULCA workgroup discussion they created a demand-to-availability ratio (DTA) in order to get better answer from previous ratios, WTA and CTA. DTA was accepted from more than half of LCA experts from many organizations (Boulay et al., 2017). Even though, DTA cannot show the amount of water availability, but only focus on the quantity that relates to the water used. For example, DTA ratio is 0.5 that mean half of the water is required by currently use, but ratio number cannot tell amount of water required. There were three criteria emerged during Pellston workshop in January 2016 (Boulay et al., 2017), that could correct the limitation. Three criteria consist of  $DTA_A$ ,  $DTA_X$ , and  $1/AMD$ .  $DTA_A$  is the same ratio but include an impact from arid locations.  $DTA_X$  consists of two parameters, one representing the DTA and the other one representing the absolute availability ( $AA_V$ ) per unit of interest area. The last one is inversion of availability minus demand ( $1/AMD$ ). Details in each criterion are shown in Table 2.6.

**Table 2.6** Evaluation results and criteria of  $DTA_X$  and  $1/AMD$  (Boulay et al., 2017)

Criteria	$DTA_A$	$DTA_X$	$1/AMD$
Description	$DTA_A = \left( \frac{Demand}{Availability} \right)$	$DTA_X = \left( \frac{Demand}{Availability} \right) \times \left( \frac{Demand}{Availability} \right)^{0.34}$	$1/AMD = \frac{Area}{Availability - Demand}$ for Demand < Availability $1/AMD = Max$ for Demand $\geq$ Availability
Pre-selection criteria of relevance regarding the question to be answered	Poor	Good	Good
Stakeholders acceptance	Option eliminated by the working group in the pre-selection process and not further investigated	Low (3/33) Only academics	Good (26/33) Academics, industry, consultants, and government
Robustness with closed basins		Limpopo shows higher scarcity (ranking and absolute value percentile)	Ganges, Yellow river, Murray, Darling, Colorado, Nile, Jordan, Indus, Syr Darya and Amu Darya, and Cauvery show higher scarcity (ranking and absolute value percentile)
Main normative choice		Absolute and relative availability have equal contribution to impacts ( $x = 0.34$ )	Regions where demand $\geq$ availability are set as maximal (equation is discontinuous)
Physical meaning		Two physical quantities, empirically combined in an index with no physical units (physical meaning for 0% of world surface)	Express a physical meaning up to the point where demand $\geq$ availability (physical meaning for 88% of world surface, monthly)

From Table 2.6  $1/AMD$  is selected for calculating in the impact of water consumption at midpoint level in LCA by based on available water remaining (AWARE : Available WATER REMaining) per unit area of water used and relative to

the world average. This criterion was created on the assumption that other users can get a result of water scarcity from the inventory data by the characterization factor,  $CF_{\text{AWARE}}$ .

$$\begin{aligned} CF_{\text{AWARE}} &= 0.1 = \text{Min} && ; \text{AMD}_i > 10 \times \text{AMD}_{\text{world avg}} \\ CF_{\text{AWARE}} &= \text{AMD}_{\text{world avg}} / \text{AMD}_i && ; \text{Demand} < \text{Availability} \\ CF_{\text{AWARE}} &= 100 = \text{Max} && ; \text{Demand} > \text{Availability or} \\ &&& \text{AMD}_i < 0.01 \times \text{AMD}_{\text{world avg}} \end{aligned}$$

$\text{AMD}_{\text{world avg}}$  is world average of available minus demand

$\text{AMD}_i$  is available minus demand value in country i

Then  $CF_{\text{AWARE}}$  is known user can get a water scarcity footprint with the following equation.

$$\text{Water Scarcity Footprint} = \text{Water consumption} \times CF_{\text{AWARE}} \quad (5)$$

### 2.4.3 Ecological Footprint

Today, world's population more than 80 percent lives in their countries that are running out of ecological resource, deficits of biocapacity (BC), because they using more resources than environmental can renew. Over the past decades, extremely decline of biocapacity occurred by human and rapidly growth of industrials. Biocapacity is the productive area available in each country or the world or another implication of biocapacity is the productive area that can regenerate annually or period of interested. Reasonwhy at the early 90s, severals environmental indicator have been developed in order to balance between humanity's demand and biocapacity. Ecological footprint (EF) is one of the environmental indicator that had been developed. The ecological footprint measures the area used to support an individual or all activities which consumes and to absorb the waste, generated from any human's event or human demand on nature. A global hectare (gha) and biocapacity are units used to express the result from ecological footprint by gha is unit for measuring human's demands on the earth and biocapacity is the ability of the earth to supply human's demands. Moreover there are many factors should be considered during assessment because in each country there are different of weather, geography, and amount of population. Ecological footprint, biocapacity, and related value can calculate by the following equations (Borucke et al., 2013).

Ecological footprint (EF) value can calculate by the following equation.

$$EF = \sum_i^n \frac{P_i}{Y_{w,i}} \times EQF_i \quad (6)$$

$P_i$  is the consumed amount of specific product  $i$  (t/yr)

$Y_{w,i}$  is the average annual yield of product  $i$

$EQF_i$  is the equivalence factor for the land use type of product  $i$ . (EQF is used to convert different particular land use types into a comparable unit, global hectares)

Biocapacity (BC), used to measure the amount of available ecological area to provide human's demand, can calculate by the following equation.

$$BC = \sum_i^n A_{N,i} \times YF_{N,i} \times EQF_i \quad (7)$$

$A_{N,i}$  is the biological area available for the production of product  $i$

$YF_{N,i}$  is the specific yield factor for the land producing of product  $i$  in each country

Yield factor (YF) can calculate by the following equation.

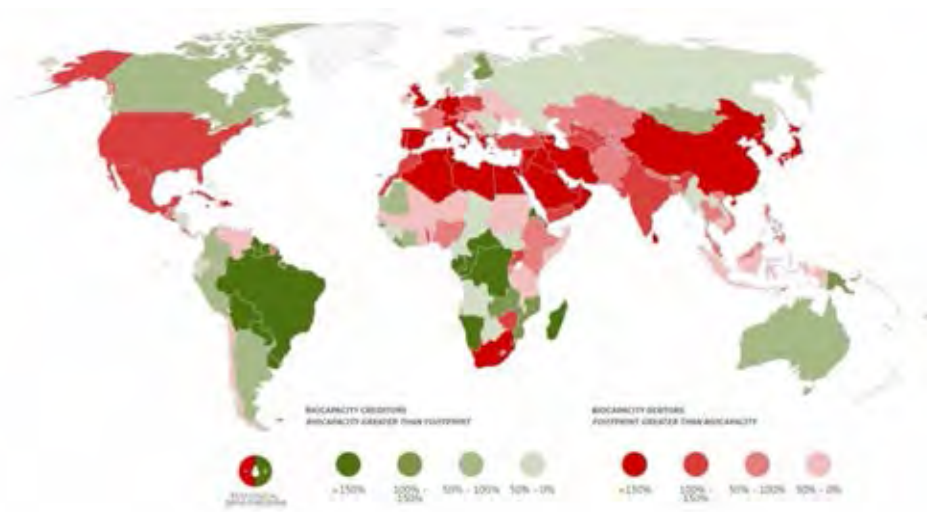
$$YF = \frac{Y_L}{Y_W} \quad (8)$$

$Y_L$  is the average local yield for land use of the same product of  $Y_W$ .

$Y_W$  is the world average yield for land use of the same product of  $Y_L$ .

Global Footprint Network group has a vision in advancing the science of sustainability. They have studied about ecological footprint. Global Footprint Network said ecological footprint is the metric to measure and compare between human's demand and natural source available. This footprint can improve or help in many ways such as, improve sustainability and optimize public project in each country moreover it can help people to understand their impact on the earth. This ecological footprint divide the land used into six different categories of productive areas. Six categories are cropland, grazing land, fishing grounds, built up land, forest

area, and carbon demand on land. Ecological footprint and biocapacity data always change every year because this value depends on the area and human population, so this data needed to update every year. Global Footprint Network collected data, which is data in 2013, of ecological footprint and biocapacity in different countries. Comparison of ecological footprint and biocapacity is shown in Figure 2.6.



**Figure 2.6** Ecological footprint and biocapacity in each country (Global Footprint Network)

As mentioned before, there are two keywords of ecological footprint, ecological footprint and biocapacity. In order to compare situation of ecosystem biocapacity need to be compared with ecological footprint value by using the same unit. There are the same and different unit between two keywords, which are shown in Table 2.7.

**Table 2.7** Unit of biocapacity and ecological footprint

Ecological Footprint Keyword	Ecological Footprint Unit
Biocapacity	- gha per person - gha
Ecological Footprint	- gha per person - gha - Number of Earths

## 2.5 Review of LCSOft Software

LCSOft is the software that used to calculate in LCA. Environmental impacts are calculated from the input data, resource, energy usage and emission. Although there are several software for calculating in LCA such as SimaPro and Gabi, LCSOft was developed in a concept of user-friendly by using Visual Basic Application (VBA) in Microsoft Excel to perform LCA calculation. Using LCSOft, users need to follow the step in software that will bring user do LCA according to framework.

The first version of LCSOft (LCSOft version 1.0) was developed by (Piyarak, 2012). The interface of LCSOft version 1.0 is easily to access and stay in a concept of user-friendly as shown in Figure 2.7.

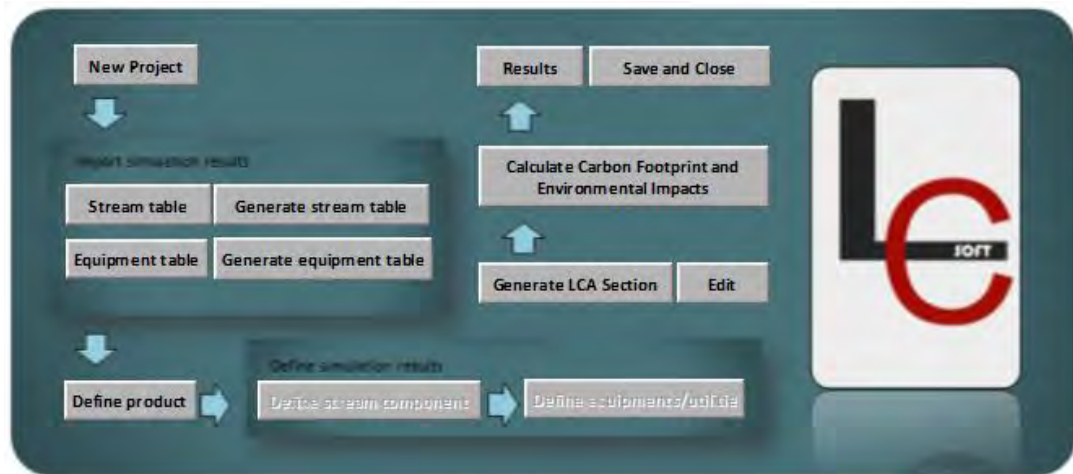


**Figure 2.7** Interface of LCSOft version 1.0 (Piyarak, 2012).

In this version consists of thirteen inventory data, energy and fuel consumption, eight environmental impacts categories, including with acidification, global warming, ozone depletion, eutrophication, photochemical formation, human toxicity, aquatic toxicity and terrestrial toxicity, and carbon footprint calculation. This version could cooperate with PROII software for calculate environmental impacts from chemical and biochemical processes. Although LCSOft interface is easy

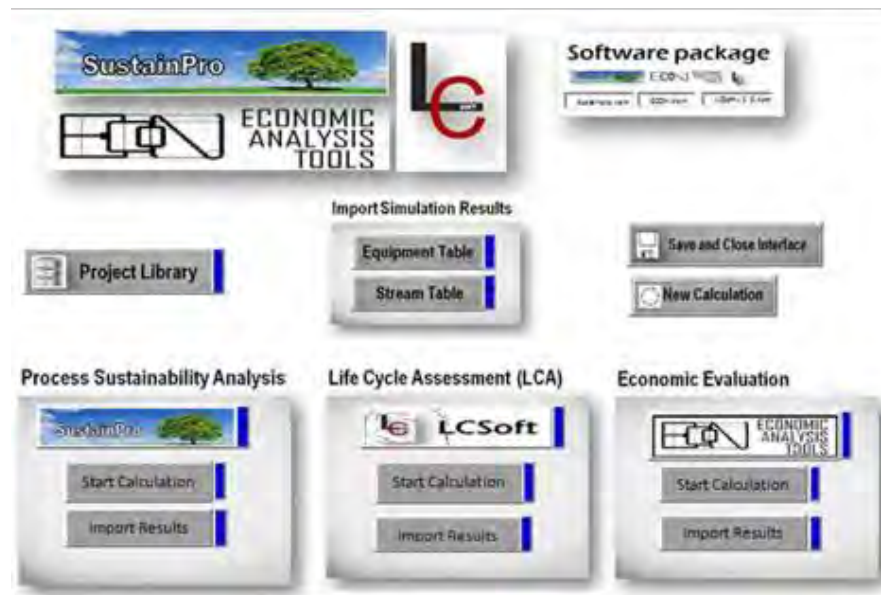
for user there are just thirteen substances in database. Therefore more data are required in LCSOft database.

The second version of LCSOft (LCSOft version 2.0) was developed by (Kalakul et al., 2014). For this version LCSOft was not only developed in its performance but also improved more function in this program. Others process design tools were integrated with LCSOft software. ECON (Saengwirun, 2011) is software for economic analysis and SustainPro is a program for sustainable process design, both of them were added into a new application of LCSOft. Figure 2.8 and 2.9 show the interface of LCSOft version 2.0 and integrated software in LCSOft respectively.



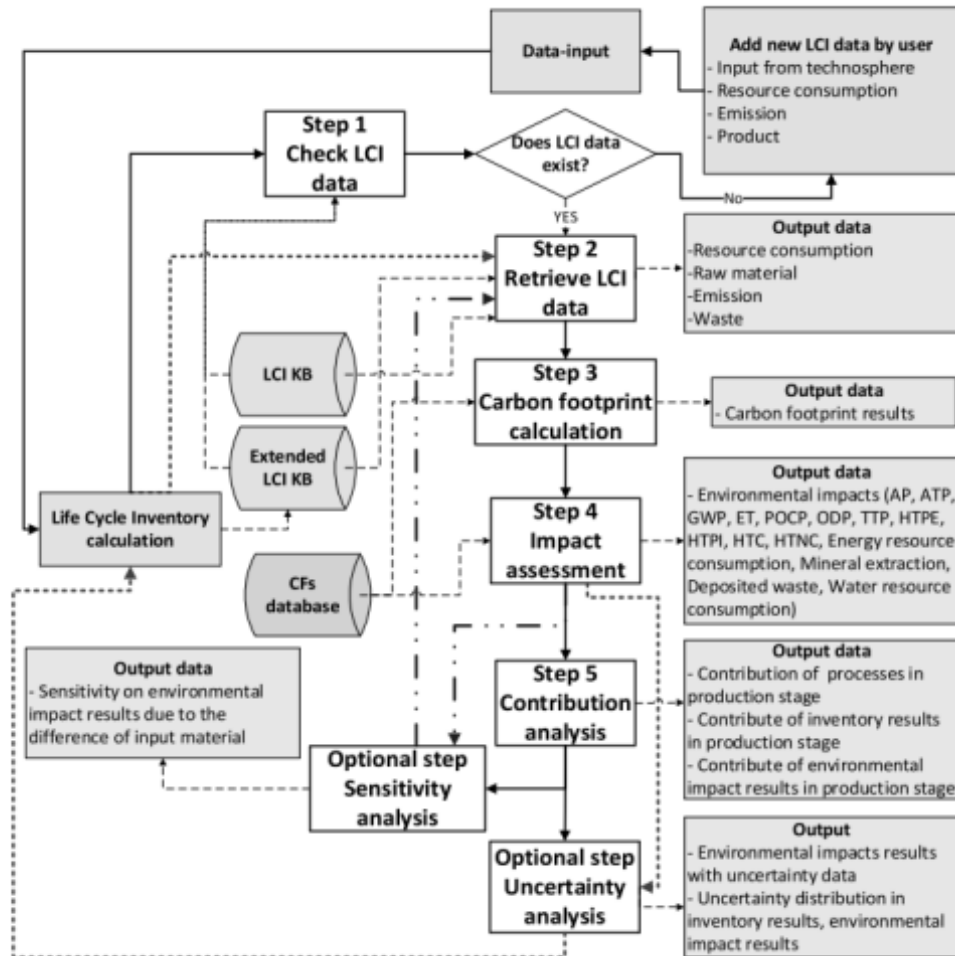
**Figure 2.8** Interface of LCSOft version 2.0 (Kalakul et al., 2014).





**Figure 2.9** Integrated Software in LCSOFT version 2.0 (Kalakul et al., 2014).

The third version of LCSOFT (LCSOFT version 3.0) was developed by (Supawanich, 2015). Development in this version consists of matrix base method (Heijungs & Suh, 2002) is used in Life Cycle Inventory calculation and more impact categories, water consumption, deposited waste, mineral extraction, and renovated energy consumption, were added. There are more functions in this version, contribution and uncertainty analysis function which is based on Monte Carlo simulation and this version also extended database by complied database from U.S. LCI and others available databases. There are five steps and two optional steps of calculation in third version of LCSOFT as shown in Figure 2.10.



**Figure 2.10** Steps of LCSoft version 3.0 (Supawanich, 2015).

The fourth version of LCSoft (LCSoft version 4.0) was developed by (Kaesinee, 2015). Extending the LCI database and there are more new impact categories were added, ionizing radiation, marine eutrophication, terrestrial eutrophication, freshwater eutrophication, photochemical ozone formation, and particular matter. Moreover, eco-efficiency which is new function was added into LCSoft for evaluated value or cost that related to the environmental which effect from product and characterization factors and unit for all impact categories in LCSoft which shown in Table 2.8.

**Table 2.8** Characterization factors and unit of general impact categories, LCIA methodology, in LCSoft (Kaesinee, 2015)

Impact Category ( $I^k$ )	Characterization factor ( $CF_{t,c}^k$ )	Unit	CF source
Acidification	$CF_{t,c}^{AP}$	kg H <sup>+</sup> eq.	USEPA
Aquatic toxicity	$CF_{t,c}^{ATP}$	1/LC <sub>50</sub>	
Global warming potential	$CF_{t,c}^{GWP}$	kg CO <sub>2</sub> eq.	
Photochemical oxidation	$CF_{t,c}^{POCP}$	kg C <sub>2</sub> H <sub>2</sub> eq.	
Ozone depletion	$CF_{t,c}^{ODP}$	kg CFC-11 eq.	
Terrestrial toxicity	$CF_{t,c}^{TTP}$	1/LD <sub>50</sub>	
Human toxicity by exposure	$CF_{t,c}^{HTPE}$	1/TWA	
Human toxicity by ingestion	$CF_{t,c}^{HTPI}$	1/LD <sub>50</sub>	
Fresh water ecotoxicity	$CF_{t,c}^{ET}$	kg 2,4-D eq.	USEtox <sup>TM</sup>
Human toxicity-carcinogenics	$CF_{t,c}^{HTC}$	kg benzene eq.	
Human toxicity-noncarcinogenics	$CF_{t,c}^{HTNC}$	kg toluene eq.	
Energy resource consumption	$CF_{t,c}^{Energy}$	MJ eq.	Cumulative Energy Demand 1.05
Mineral extraction	$CF_{t,c}^{Mineral}$	kg Sb eq.	CML-IA
Deposited waste	$CF_{t,c}^{Waste}$	UBP	Ecological scarcity 2013
Water resource consumption	$CF_{t,c}^{Water}$	UBP	
Photochemical ozone formation	$CF_{t,c}^{PCOF}$	kg NMVOC eq.	ILCD2011
Marine eutrophication	$CF_{t,c}^{Marine}$	kg N eq.	
Freshwater eutrophication	$CF_{t,c}^{Freshwater}$	kg P eq.	
Terrestrial eutrophication	$CF_{t,c}^{Terrestrial}$	mol N eq.	
Ionizing radiation	$CF_{t,c}^{IR}$	kbq U <sub>235</sub> eq.	
Particular matter	$CF_{t,c}^{PM}$	kg PM <sub>2.5</sub> eq.	

The fifth version of LCSoft (LCSoft version 5.0) was developed by (Chavewanmas, 2016). Improvement on LCI and LCIA in this version by adding new pathway calculation and allocation, the reports from case study gave more accuracy results. New features also been added in to software consists of normalization, data quality indicator, parameter sensitivity analysis, ILCD midpoint impact categories and uncertainty. LCI database was extended to cover all calculation of impact categories. Environmental impact categories of ILCD methodology are shown in Table 2.9.

**Table 2.9** Environmental impact categories and unit of ILCD methodology

ILCD 2011 Impact Categories	Unit
Global Warming	kg CO2 eq
Ozone Depletion	kg CFC-11 eq
Human toxicity, cancer effect	CTUh
Human toxicity, non-cancer effect	CTUh
Fresh Water Ecotoxicity	CTUe
Particulate matter	kg PM2.5 eq
Ionizing radiation	kg U235 eq
Photochemical Ozone Formation	kg NMVOC eq
Acidification	molc H+ eq
Terrestrial eutrophication	molc N eq
Freshwater eutrophication	kg P eq
Marine eutrophication	kg N eq
Water Resource Consumption	m3 water eq
Mineral Extraction	kg Sb eq
Land use	kg C deficit

**Methods**

General Impact Categories

General Impact Categories is a LCIA methodology developed by LCSOFT's team

This LCIA methodology includes 21 midpoint impact categories

- 1-Acidification
- 2-Aquatic toxicity
- 3-Global warming potential
- 4-Photochemical oxidation
- 5-Ozone depletion
- 6-Terrestrial toxicity
- 7-Human toxicity by exposure
- 8-Human toxicity by ingestion
- 9-Fresh water ecotoxicity

Including uncertainty in calculation

%  uncertainty

**Figure 2.11** Uncertainty feature in LCSOFT version 5.0 (Chavewanmas, 2016).

**Figure 2.12** Parameter Sensitivity Analysis in LCSOFT version 5.0 (Chavewanmas, 2016).

## 2.6 Carbon Dioxide Capture and Utilization (CCU) Process

The increment of CO<sub>2</sub> in atmosphere become a big chain problem because of carbon dioxide emission from daily routine of human activities. Reason why there are many alternative ways and technologies to decrease CO<sub>2</sub> emission from different emission sources, using alternative or green energy instead of using fossil fuel energy, for example using solar energy, wind energy, thermal energy, hydro power, and etc., and using technologies to capture CO<sub>2</sub> and using them for others benefit. Around 40 percent of CO<sub>2</sub> emission which related to the fossil fuel come from the power plant and most of the rest come from industries. Carbon dioxide capture and utilization process (CCU) is continuously developed in order to solve this problem. CCU is process that makes an effort to reduce carbon dioxide emissions by using them in commercial products. The concept of CCU process is capturing CO<sub>2</sub> from any kind of industrial plant and convert captured CO<sub>2</sub> into a commercial product

(Wiesberg et al., 2017). There are many technologies to capture CO<sub>2</sub> such as physical solvents, chemical solvents, membrane separation, and adsorption (Rostami Dehjalali & Avami, 2017). Moreover, CO<sub>2</sub> can be used as raw material for a variety of product and others function in industrial. For example, dimethyl carbonate and ethylene glycol are a widely use chemical can be produce by using CO<sub>2</sub> as raw material. Gas injection, CO<sub>2</sub>, is one of the various techniques for increasing amount of crude oil produced in petroleum industry.

### 2.6.1 Dimethyl Carbonate (DMC)

Dimethyl Carbonate (DMC), with formula (CH<sub>3</sub>O)<sub>2</sub>CO, is an important chemical intermediate and also environmental friendly. The annual demand rate of DMC is continue increasing every year in the past decade with more than 90,000 tons per year of DMC is consumed (Pyo et al., 2017). DMC become as a famous intermediate chemical because it can use with broader range of industrial application. For example, around 50 percent of DMC is used in inks, paints, coating, electrolyte in ion-battery, and as intermediate, 25 percent in polymer synthesis, antioxidant, resins, pharmaceuticals, and pesticides. There are different ways to produce DMC in industrial scale, e.g., tranesterification, phosgene, and the oxidative carbonylation of methanol, which still have been developed. In term of sustainable development and environmental friendly the latest way, the oxidative carbonylation of methanol, is very famous because this process synthesis of DMC by utilizing CO<sub>2</sub>, waste from other processes, as raw material. CO<sub>2</sub> emission to environmental from other processes, coal, petroleum, and chemical industrial, is captured by CCU process and feeded as raw material into DMC production process. DMC can produce by reaction between CO<sub>2</sub> and methanol (Tan et al., 2018).

### 2.6.2 Ethylene Glycol (EG)

Ethylene glycol (EG) is the simplest diol with the formula (CH<sub>2</sub>OH)<sub>2</sub>. In 2014, around 25 million tons of EG were needed for industrial and the trend of using EG also continues to grow with annual increasing rate around 5 percent (Lu et al., 2018). EG is the widely used for automobile engine coolants, antifreezes and de-icer sprayed on airplane wing and on runway of airport to prevent them freezing in

winter moreover its largest use in film and polyester manufacturer. EG is also used in paints, surfactants, heat transfer fluid, emulsifiers, and hydraulic fluids (Carney & Stice, 2017). EG is produced from carbon dioxide as a raw material with ethylene oxide as an intermediate. Ethylene oxide react with water to produce ethylene glycol. However, excess of water is required during the synthesis of EG in order to inhibit the unexpected product of di-ethylene glycol and tri-ethylene glycol.

## **CHAPTER III**

### **METHODOLOGY**

#### **3.1 Materials and Equipment**

##### 3.1.1 Equipment

- Notebook, Asus A43S, Intel® Core™ i5-2450M CPU @ 2.50GHz, 8.0 GB of RAM
- All In One PC, Acer, Intel® Core™ i7-3770S CPU @ 3.10GHz, 8.0 GB of RAM

##### 3.1.2 Software

- LCSOFT
- Microsoft Excel 2010
- Visual Basic for Application
- SimaPro v.8.3
- Windows 7 Enterprise, Copyright © 2009 Microsoft Corporation, All rights reserved

#### **3.2 Methodology**

##### 3.2.1 Adding Equipment and Column Conditions

In order to comprehend more complexity and wider range of application used in new sustainable process designed, new equipment and more column condition are added in this version of LCSOFT. Compressor is added as new equipment in LCSOFT and some column which has only condenser or reboiler, new condition of column, can calculate by the latest version of LCSOFT.



### 3.2.2 Adding New LCIA Methodologies

In previous version, LCSOFT version 5.0, there are two midpoints and one endpoint of LCIA methodologies consist of general impact categories and ILCD 2011, developed by LCSOFT's team and Joint Research Centre of European Commission respectively. In order to improve performances, wider applications range and flexibilities, this version covers all levels of LCA impact by adding new LCIA methodologies into method selection. New LCIA methodologies consist of ReCiPe midpoint and ReCiPe endpoint. ReCiPe was developed by RIVM.

### 3.2.3 New Environmental Footprint in Interpretation

Each environmental footprint is used to assess the specific situation of environment. Previous version of LCSOFT has only carbon footprint to measure the total amount of greenhouse gas, expressed in kg CO<sub>2</sub>. In order to cover more perspectives of environment, other environmental footprints are added into the latest version of LCSOFT. New environmental footprints in LCSOFT are water scarcity footprint and ecological footprint, added as an optional function of interpretation.

#### 3.2.3.1 *Water Scarcity Footprint*

In the ISO 14046, a water footprint is used as an indicator to assess freshwater of production process, which is a part of LCA. To this day, none of consensus water footprint method that consider about different scarcity of water in different country and a period of time. Water Scarcity Footprint, developed by Water Use in Life Cycle Assessment (WULCA), consensus model which its characterization factors related to scarcity of water in different country and a period of time, is added into LCSOFT as an optional function of interpretation. Water Scarcity Footprint can be calculated by using characterization factor and amount of water used in process by eq. (5).

#### 3.2.3.2 *Ecological Footprint*

The purpose of ecological footprint is assessment of area used to support an individual or all activities which consumes and to absorb the waste, generated from any event. Normally, ecological footprint is expressed as global hectares, global hectares per person and biocapacity. Each ecological footprint assessment depends on the location because there are different of resource,

geography, climate and population in each country. This ecological footprint is expressed in different purpose of land used, such as built up land, cropland, carbon, forest products, and grazing.

#### 3.2.4 Validation and Improvement of LCSoft

The validation of results is the step for check some errors and accuracy from LCSoft software by compare result from the same processes with another LCA software, SimaPro. In order to represent the ability and efficiency of LCSoft, results from LCA calculation of bioethanol from cassava rhizome and a dimethyl carbonate from carbon dioxide capture process are validated by comparing with SimaPro.

## **CHAPTER IV**

### **RESULTS AND DISCUSSION**

#### **4.1 Adding Equipment and Column Conditions**

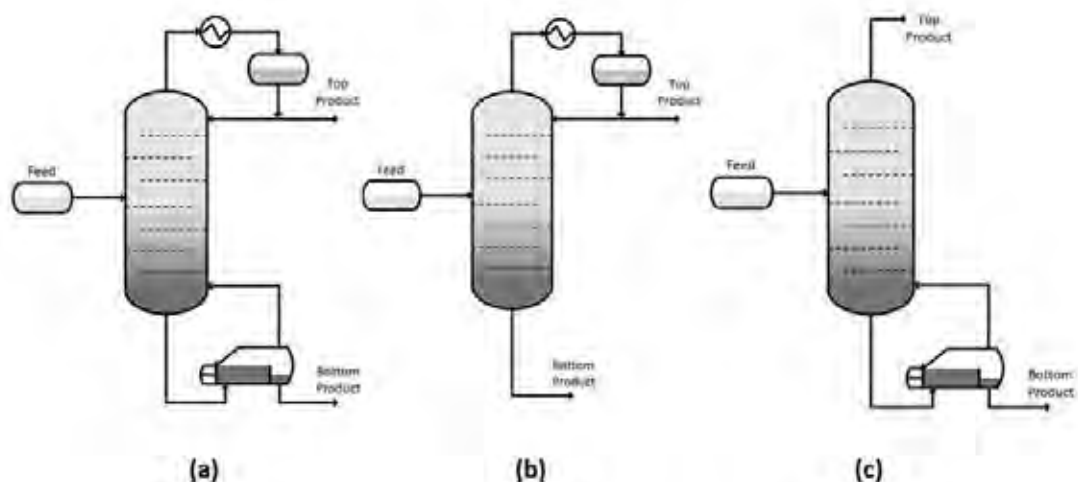
There are much equipment and technologies in petroleum, petrochemical and others process. For catch up new industrial technology, LCSofT is improved and developed in order to cover all essential equipment and more unit conditions.

##### 4.1.1 Adding Essential Equipment

Equipment is an important element in any kind of process. Most of them are a main factor of environmental impact calculated by LCA software because a lot of energy is consumed by that equipment. For comprehend and efficiency to assess environmental impacts some equipment which not available in previous version of LCSofT is added in the latest version. Compressor is common equipment in industrial and uses a lot of energy which cause a main factor of environmental impact, but it is not provide in previous version, so it is added in this version already.

##### 4.1.2 Adding Column Conditions

Column unit consists of reboiler and condenser at bottom and top of column respectively, normally during the operation condenser and reboiler are used at the same time in order to distillate for pure product. However, there are many techniques and design for industrial to reduce operating and investment cost, some technique column is operated with only condenser or reboiler, which LCSofT cannot assess the environmental for this condition reason why this condition is added into LCSofT. So, in the latest version of LCSofT can calculate environmental impact from column unit which has both condenser and reboiler or only condenser or reboiler, different operating of column conditions are shown in Figure 4.1. After more conditions of column are added into software, LCSofT can assess environmental impact more precisely.



**Figure 4.1** Types of column (a) column with condenser and reboiler (b) column with only condenser (c) column with only reboiler.

## 4.2 New LCIA Methodologies for Calculation

Previous LCSOFT version has two LCIA categories, in method selection, for LCA calculation, general impacts categories and ILCD 2011, both of them are midpoint impact level and endpoint impact level for ILCD 2011. For general impact categories method in LCSOFT, this method has twenty-one impact categories consist of different characterization factor of environmental impact from different sources, fifteen midpoint impact categories and three endpoint impact categories in ILCD 2011 (Chavewanmas, 2016). Comparison of LCIA methodologies between previous version and latest version is shown in Table 4.1. In order to cover wider range of user, new midpoint and endpoint impact categories are added as choices in LCIA method selection consist of ReCiPe midpoint and ReCiPe endpoint.

**Table 4.1** Comparable of LCIA methodologies in LCSoft

Impact level	LCIA methodologies in LCSoft	
	Previous version	Latest version
Midpoint	General Impact categories ILCD 2011	General Impact categories ILCD 2011 ReCiPe (Egalitarian) ReCiPe (Individualist) ReCiPe (Hierarchist)
Endpoint	ILCD 2011	ILCD 2011 ReCiPe (Egalitarian) ReCiPe (Individualist) ReCiPe (Hierarchist)

From Table 4.1, for sustainable development each ReCiPe method, midpoint and endpoint, contains factors according to three different cultural perspectives. Different perspectives represent like a choices for interesting situation, time or expectations from user. Three perspectives consist of egalitarian, individualist, and hierarchist all of this perspective are defined in the following lists.

Egalitarian (E) always used for long term consideration which based on precautionary statements.

Individualist (I) is based on short term analysis, which user always looking on a good side that many problems in future can avoided by present technology.

Hierachist (H) is based on scientific models, so this model is considered as a default or consensus model for LCA calculation of ReCiPe method.

However, all perspective level, E, I, and H, in midpoint and endpoint of ReCiPe method are different in meaning and purpose of using. There are the same amounts of environmental impacts that are considered by ReCiPe. For ReCiPe methodology, LCA results are determined with two levels, eighteen impacts for midpoint and three impacts for endpoint, which are shown in Table 4.2 and 4.3 respectively.

**Table 4.2** Environmental impact categories and unit of ReCiPe midpoint methodology

ReCiPe (E,H,I) midpoint Impact Categories	Unit
Climate Change	kg CO2 eq.
Ozone Depletion	kg CFC-11 eq.
Terrestrial Acidification	kg SO2 eq.
Freshwater Eutrophication	kg P eq.
Marine Eutrophication	kg N eq.
Human Toxicity	kg 1,4-DB eq.
Photochemical Oxidant Formation	kg NMVOC
Particulate Matter Formation	kg PM10 eq.
Terrestrial Ecotoxicity	kg 1,4-DB eq.
Freshwater Ecotoxicity	kg 1,4-DB eq.
Marine Ecotoxicity	kg 1,4-DB eq.
Ionising Radiation	kg U235 eq.
Agricultural Land Occupation	m2a
Urban Land Occupation	m2a
Natural Land Occupation	m2a
Water Depletion	m3
Metal Depletion	kg Fe eq.
Fossil Depletion	kg oil eq.

**Table 4.3** Environmental impact categories and unit of ReCiPe endpoint methodology

ReCiPe (E,H,I) endpoint Impact Categories	Unit
Ecosystem	species/yr
Human Health	DALY
Resources	\$

### 4.3 New Environmental Footprint in Interpretation

In order to achieve many environmental policies, two new environmental footprints are added into this version of LCSoft as an optional function in interpretation step. New footprints consist of water scarcity footprint and ecological footprint.

#### 4.3.1 Water Scarcity Footprint

Water Scarcity Footprint (Boulay et al., 2017) is a consensus model used to evaluate water scarcity of interesting product. Several specific conditions are considered in this model, so there is different characterization factors for each condition, such as scarcity of water in different time period, country, and purpose of water used. Water scarcity footprint is added as a new optional function of interpretation in LCSof. Moreover users can select the types or purpose (as shown in Table 4.4) of water used, consist of agricultural, non-agricultural, and unspecified, on a new project window of LCSof. After environmental impacts calculation, user needs to input amount of water used for the process with the same flow rate that selected on a new project window.

**Table 4.4** Types of water selection choices in LCSof

Types or purposes of water use for each process
Agricultural
Non-Agricultural
Unspecified

#### 4.3.2 Ecological Footprint

Ecological footprint is provided as an optional function in this version of LCSof. Ecological footprint measures the demand on nature and how much nature we have on the planet. This will help each country improve their policy for sustainability, minimize project investment in each local, and help population understand with their impact on the earth. Ecological footprint in LCSof is expressed in area, hectares. In order to ease understand by user there are different of ecological footprint unit show in Table 4.5.

**Table 4.5** Ecological footprint unit available in LCSOft

Unit of Ecological Footprint
Biocapacity (gha per person)
Biocapacity (gha)
Ecological Footprint (gha per person)
Ecological Footprint (gha)
Ecological Footprint (Number of Earths)

#### 4.4 Validation and Improvement of LCSOft

In the latest version of LCSOft, new features and improvements function are added into software. Furthermore new version of LCSOft was validated with commercial LCA software, SimaPro version 8.3, in order to compare the environmental impact assessment results through case studies. There are two cases study are assessed the environmental impacts by LCSOft and compared with SimaPro version 8.3. In order to prove that LCSOft has an ability to assess environmental impacts from any kind of process, so these two case studies are selected as case study bioethanol product from cassava rhizome (biochemical process) and dimethyl carbonate produced from carbon dioxide capture and utilization processes, CCU process, (petrochemical process). LCIA methodologies are used to evaluate environmental impacts for each process is shown in Table 4.6.

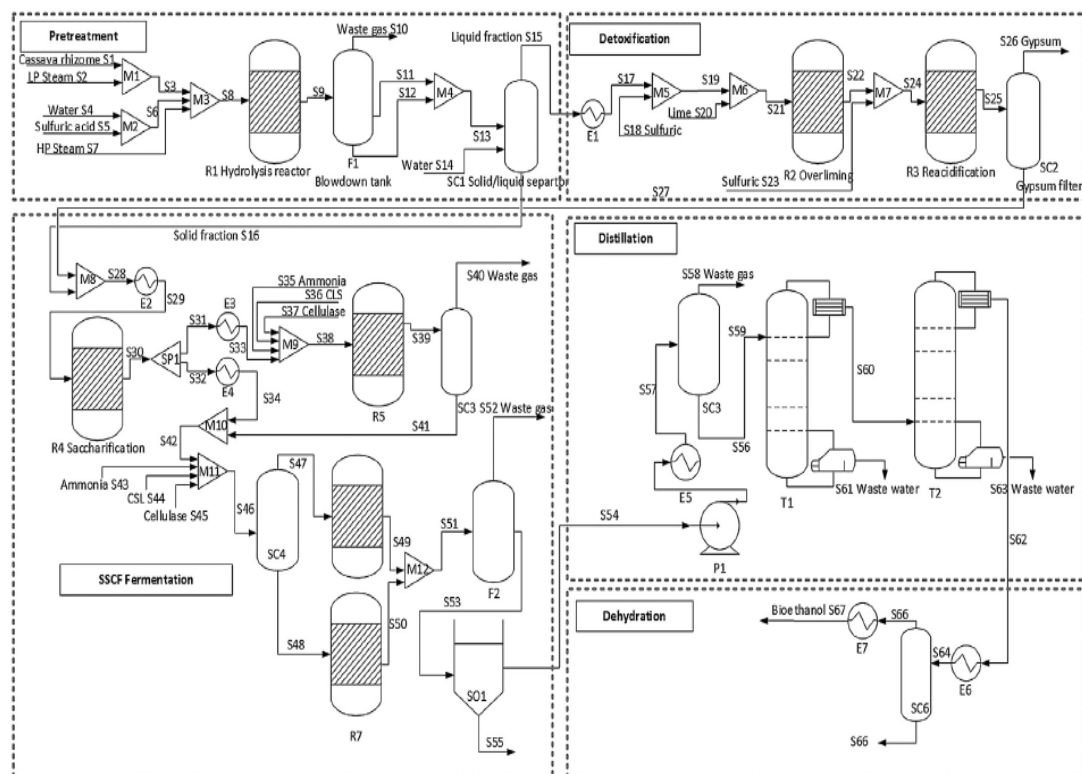
**Table 4.6** Processes and LCIA methodologies used for environmental assessment

Process	LCIA method
Bioethanol from cassava rhizome	ReCiPe (H) midpoint
	ReCiPe (H) endpoint
Dimethyl carbonate from carbon dioxide capture processes	ReCiPe (I) midpoint
	ReCiPe (I) endpoint



#### 4.4.1 Bioethanol from Cassava Rhizome

The life cycle assessment of bioethanol produced from cassava rhizome is focused from production of cassava phase, transportation, and manufacturing or the scope of this study is cradle-to-gate. Data in this process were taken from the process simulation (Mangnimit, et al., 2013), process flow sheet is shown in Figure 4.2.



**Figure 4.2** Bioethanol from cassava rhizome process flow sheet.

119 tons/day of bioethanol product are produced in the process 377 tons/day of biomass inputted and 1 kg of pure ethanol is considered for LCA study of this process. Others contribution, Materials are: Ammonia (steam reforming liquid at plant), Cassava root, Corn steep liquor, Enzyme Cellulase Novozyme Celluclast, and Sulfuric acid (at plant). Utilities are: Chilled water (engine-driven chiller using natural gas), Electricity (natural gas, at power plant), and Natural gas (combusted in industrial equipment), of bioethanol process are shown in Table 4.7.

**Table 4.7** Contribution of bioethanol process

Contribution of Bioethanol Process	Amount	Unit
<i>Material</i>		
Ammonia, steam reforming, liquid, at plant	3.31	kg
Cassava root	15008.13	kg
Corn steep liquor	147.47	kg
Enzyme, Cellulase, Novozyme, Celluclast	8.32	kg
Sulfuric acid, at plant	258.34	kg
<i>Utility</i>		
Chilled water, engine-driven chiller using natural gas	47938.30	MJ
Electricity, natural gas, at power plant	5.70	kWh
Natural gas, combusted in industrial equipment	60584.60	MJ

In order to compare the environmental result between LCSOft and SimaPro, bioethanol process is used as one of case study for compare the environmental result and for this case ReCiPe (H) midpoint and endpoint are used as LCIA method for LCA calculation, which ReCiPe method is available in the latest of LCSOft and SimaPro version 8.3.

The material and utility shown in Table 4.7, which contained in LCI database of LCSOft by they are obtained from US.LCI and others literature, are selected in order to analyze the environmental impacts.

For SimaPro, the same materials and utilities selected in LCSOft are also used in SimaPro, but in SimaPro some materials are not existed. Reason why Cassava rhizome, Corn steep liquor, and Enzyme Cellulase Novozyme Celluclast are performed by using LCI data based on literature.

Environmental impacts result by using bioethanol from cassava rhizome process as a case study with 18 midpoint and 3 endpoint impact categories from ReCiPe (H) for LCIA methodology are shown in Table 4.8. The results from the latest version of LCSOft and SimaPro version 8.3 are in the same trend of LCA calculation. However, there are slightly different in each environmental impact, but the different in each impact is in the acceptable range. For freshwater ecotoxicity and human toxicity have a wider gap different between LCSOft and SimaPro than other impacts because US.LCI database in LCSOft has smaller sets of emission

factors from combustion fuel. Database in LCSoft also has larger set of consuming fossil fuel, so fossil depletion impact calculated by LCSoft has slightly higher effect than the result calculated by SimaPro. Whatever, almost whole environmental impact results are closely and the different results between LCSoft and SimaPro are in the acceptable range.

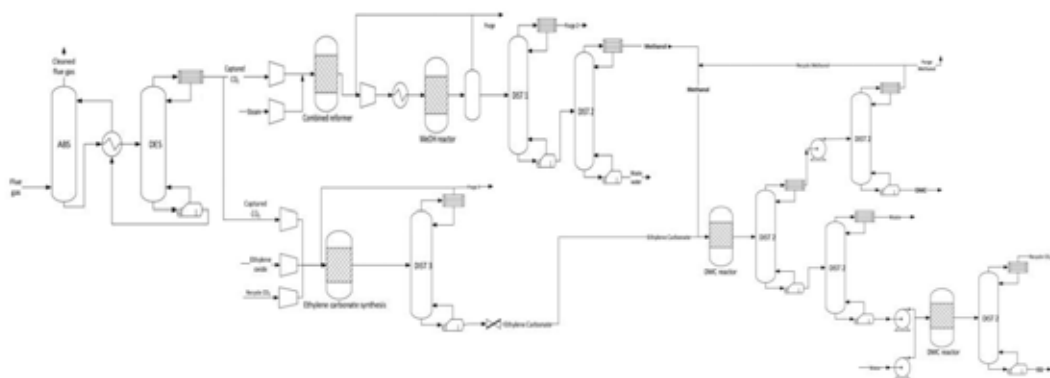
**Table 4.8** Comparison result of bioethanol from cassava rhizome process using ReCiPe (H) midpoint and endpoint

Impact Categories	Unit	LCSoft	SimaPro
<i>ReCiPe Midpoint</i>			
Climate Change	kg CO2 eq.	2.31133	2.36460
Ozone Depletion	kg CFC-11 eq.	1.61E-12	1.73E-12
Terrestrial Acidification	kg SO2 eq.	0.00362	0.00959
Freshwater Eutrophication	kg P eq.	5.18E-06	5.18E-06
Marine Eutrophication	kg N eq.	0.00012	0.00014
Human Toxicity	kg 1,4-DB eq.	0.00369	0.16753
Photochemical Oxidant Formation	kg NMVOC	0.00213	0.00263
Particulate Matter Formation	kg PM10 eq.	0.00077	0.00196
Terrestrial Ecotoxicity	kg 1,4-DB eq.	3.96E-07	5.35E-07
Freshwater Ecotoxicity	kg 1,4-DB eq.	0.00045	0.00211
Marine Ecotoxicity	kg 1,4-DB eq.	0.00118	0.00195
Ionising Radiation	kg U235 eq.	0.00E+00	0.00E+00
Agricultural Land Occupation	m2a	0.00E+00	0.00E+00
Urban Land Occupation	m2a	0.00E+00	0.00E+00
Natural Land Occupation	m2a	0.00E+00	0.00E+00
Water Depletion	m3	0.00007	0.00007
Metal Depletion	kg Fe eq.	3.82E-08	3.83E-08
Fossil Depletion	kg oil eq.	0.39005	0.31975
<i>ReCiPe Endpoint</i>			
Ecosystem	species/y	1.94E-08	1.8787E-08
Human Health	DALY	4.73E-06	3.9378E-06
Resources	\$	0.06454	0.05284

#### 4.4.2 Dimethyl Carbonate from Carbon Dioxide Capture Process

Carbon dioxide capture and utilization (CCU) process is process that make an effort to reduce carbon dioxide emission by using them in commercial

products, dimethyl carbonate is valuable and widely used product in petrochemical industrial. The life cycle assessment of CCU process focuses on gate to gate evaluation and also has some assumptions, such as this plant is located in Denmark, carbon dioxide which is raw material in this process is available from anywhere or do not concern about the previous processes that create carbon dioxide and allocation in this case study is allocated for materials and utilities in this process. Allocation in this case is based on molar flow rate of dimethyl carbonate (product) and ethylene glycol (co product). The CCU process convert carbon dioxide to valuable and widely used products dimethyl carbonate, material, and ethylene glycol, co product, involves 4 parts consist of carbon dioxide capture from another plant or available source, conversion of carbon dioxide to methanol, conversion of carbon dioxide to ethylene carbonate, and the synthesis of dimethyl carbonate from this methanol and ethylene carbonate. Moreover dimethyl carbonate is produce as a main product from this process, ethylene glycol, which is the valuable and widely used in petrochemical industry, also produced as a co product from this process.



**Figure 4.3** Carbon dioxide capture and utilization (CCU) process flow sheet.

348 tons/day of dimethyl carbonate, product, and 381 tons/day of ethylene glycol, co product, are produced in the process by using 3122 tons/day of carbon dioxide from available source as raw material and converted carbon dioxide into commercial and widely used product through the process as shown in Figure 4.3. 1 kg of pure dimethyl carbonate and 1 kg of pure ethylene glycol are considered for

LCA studies of product and co-product from this process respectively. Others contribution of raw material and utilities are used in this carbon dioxide capture and utilization (CCU) process for dimethyl carbonate, product, and ethylene glycol, co product, shown in Table 4.9.

**Table 4.9** Contribution of carbon dioxide capture and utilization process

Contribution of CCU process	Amount	Unit
<i>Material</i>		
Ethylene oxide, at plant	3.3	kg
<i>Utilities</i>		
Chilled water, engine-driven chiller using natural gas	1,252,843.59	kJ
Electricity, natural gas, at power plant	20.60	kWh
Natural gas, combusted in industrial equipment	351.11	MJ

Carbon dioxide capture and utilization process has ability to convert carbon dioxide into commercial, dimethyl carbonate (product), moreover than produce only product it also produce another commercial product, ethylene glycol is also produced as a co product, from this process. For this case study, input, output, and utilities data of this process are available. In order to assess environmental impacts from this process correctly, allocation of materials and utilities, used in this process, is required before calculate environmental impacts with LCA software. With data available of this process, assumptions of allocation are based on the following assumptions: Allocation is based on molar flow rate, kg mol per second, between dimethyl carbonate (product) and ethylene glycol (co product) as shown in Table 4.10. Materials and utilities used in this process are allocated which are shown in Table 4.11 and 4.13 for dimethyl carbonate and ethylene glycol respectively. Other assumptions of this process are the same as mentioned before.

**Table 4.10** Molar flow rate of product and co product in CCU process

Chemical	Type	Flow Rate	Unit
Dimethyl carbonate	product	0.045	kg mol/s
Ethylene glycol	co product	0.071	kg mol/s

For the calculation of environmental impact results of dimethyl carbonate (product), others contribution of dimethyl carbonate from CCU process such as material and utilities (ethylene oxide (at plant), Chilled water (engine-driven chiller using natural gas), electricity (natural gas at power plant), and natural gas (combusted in industrial equipment), which are allocated based on molar flow rate between dimethyl carbonate (product) and ethylene glycol (co product) as shown in Table 4.10. Data with allocation is used as the input data in order to assess the environmental impact by LCSofT and SimaPro, are shown in Table 4.11.

**Table 4.11** Contribution of dimethyl carbonate from CCU Process

Contribution of dimethyl carbonate from CCU process	Amount	Unit
<i>Material</i>		
Ethylene oxide, at plant	1.28	kg
<i>Utilities</i>		
Chilled water, engine-driven chiller using natural gas	484,066.28	kJ
Electricity, natural gas, at power plant	7.96	kWh
Natural gas, combusted in industrial equipment	135.66	MJ

Environmental impact results of dimethyl carbonate produced from CCU process are calculated by using ReCiPe (I) midpoint and endpoint as a LCIA methodology. Environmental impact results from both software, LCSofT and SimaPro, are in the same trend although there are some slightly different result between LCSofT and SimaPro it is in the acceptable range. Due to smaller sets of emission factors from combustion fuel of US.LCI database in LCSofT, freshwater ecotoxicity and human toxicity have a wider gap different between LCSofT and SimaPro. There is wider different gap of fossil depletion impact result calculated from LCSofT and SimaPro because CCU process use fossil fuel in operation units more than bioethanol process and set of consuming fossil fuel in LCSofT is larger than SimaPro, which already mentioned in previous case study. Reason why resources impact in endpoint impacts result calculated by LCSofT is higher than SimaPro. Whatever, almost whole environmental impact results are closely and are in the same trend. The comparing results of dimethyl carbonate by CCU process,

calculated by using ReCiPe (I) as a LCIA methodology, between LCSofT and SimaPro are shown in Table 4.12.

**Table 4.12** Comparison result of dimethyl carbonate from CCU process using ReCiPe (I) midpoint and endpoint

Impact Categories	Unit	LCSofT	SimaPro
<i>ReCiPe Midpoint</i>			
Climate Change	kg CO <sub>2</sub> eq.	80.34193	75.53734
Ozone Depletion	kg CFC-11 eq.	4.69E-12	1.98E-11
Terrestrial Acidification	kg SO <sub>2</sub> eq.	0.01016	0.03461
Freshwater Eutrophication	kg P eq.	0.00E+00	0.00E+00
Marine Eutrophication	kg N eq.	0.00032	0.00021
Human Toxicity	kg 1,4-DB eq.	0.01055	0.05499
Photochemical Oxidant Formation	kg NMVOC	0.01818	0.02282
Particulate Matter Formation	kg PM <sub>10</sub> eq.	0.00353	0.00779
Terrestrial Ecotoxicity	kg 1,4-DB eq.	3.78E-06	3.33E-06
Freshwater Ecotoxicity	kg 1,4-DB eq.	0.00361	0.00999
Marine Ecotoxicity	kg 1,4-DB eq.	0.00885	0.00908
Ionising Radiation	kg U235 eq.	0.00E+00	0.00E+00
Agricultural Land Occupation	m <sup>2</sup> a	0.00E+00	0.00E+00
Urban Land Occupation	m <sup>2</sup> a	0.00E+00	0.00E+00
Natural Land Occupation	m <sup>2</sup> a	0.00E+00	0.00E+00
Water Depletion	m <sup>3</sup>	0.00052	0.00052
Metal Depletion	kg Fe eq.	0.00E+00	0.00E+00
Fossil Depletion	kg oil eq.	4.70155	1.93979
<i>ReCiPe Endpoint</i>			
Ecosystem	species/y	9.57E-05	9.20E-05
Human Health	DALY	1.88E-06	5.99E-07
Resources	\$	0.24310	0.10044

For the calculation of environmental impact results of ethylene glycol, others contribution of ethylene glycol as a co product of dimethyl carbonate from CCU process such as material and utilities (same as dimethyl carbonate), which are allocated based on molar flow rate as shown in Table 4.10. These allocated contribution data are used as the input of material and utilities data in order to assess the environmental impact by LCSofT and SimaPro, are shown in Table 4.13.

**Table 4.13** Contribution of ethylene glycol (co product) from CCU Process

Contribution of ethylene glycol from CCU process	Amount	Unit
<i>Material</i>		
Ethylene oxide, at plant	2.02	kg
<i>Utilities</i>		
Chilled water, engine-driven chiller using natural gas	768,777.31	kJ
Electricity, natural gas, at power plant	12.64	kWh
Natural gas, combusted in industrial equipment	215.45	MJ

**Table 4.14** Comparison result of ethylene glycol (co product) from CCU process using ReCiPe (I) midpoint and endpoint

Impact Categories	Unit	LCSoft	SimaPro
<i>ReCiPe Midpoint</i>			
Climate Change	kg CO2 eq.	127.59627	119.96579
Ozone Depletion	kg CFC-11 eq.	7.45E-12	3.14E-11
Terrestrial Acidification	kg SO2 eq.	0.01614	0.05497
Freshwater Eutrophication	kg P eq.	0.00E+00	0.00E+00
Marine Eutrophication	kg N eq.	0.00051	0.00033
Human Toxicity	kg 1,4-DB eq.	0.01676	0.08733
Photochemical Oxidant Formation	kg NMVOC	0.02887	0.03624
Particulate Matter Formation	kg PM10 eq.	0.00561	0.01237
Terrestrial Ecotoxicity	kg 1,4-DB eq.	6.00E-06	5.29E-06
Freshwater Ecotoxicity	kg 1,4-DB eq.	0.00573	0.01587
Marine Ecotoxicity	kg 1,4-DB eq.	0.01406	0.01442
Ionising Radiation	kg U235 eq.	0.00E+00	0.00E+00
Agricultural Land Occupation	m2a	0.00E+00	0.00E+00
Urban Land Occupation	m2a	0.00E+00	0.00E+00
Natural Land Occupation	m2a	0.00E+00	0.00E+00
Water Depletion	m3	0.00083	0.00083
Metal Depletion	kg Fe eq.	0.00E+00	0.00E+00
Fossil Depletion	kg oil eq.	7.46684	3.08071
<i>ReCiPe Endpoint</i>			
Ecosystem	species/y	0.00015	0.00015
Human Health	DALY	2.99E-06	9.51E-07
Resources	\$	0.38608	0.15952

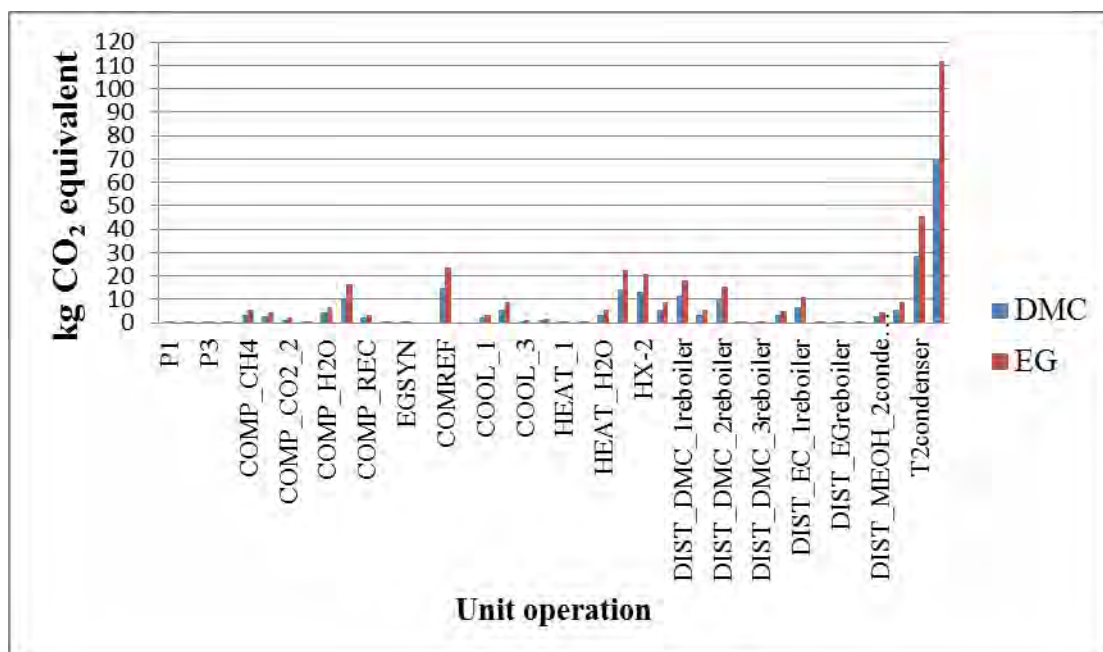


Environmental impact results of ethylene glycol produced as a co product from CCU process, shown in Table 4.14 are calculated by using ReCiPe (I) midpoint and endpoint as a LCIA methodology. After allocation, contribution of materials and utilities used to produce ethylene glycol as co product in CCU process are higher than contribution data used to produce dimethyl carbonate in CCU process, because flow rate of ethylene glycol is higher than dimethyl carbonate as shown in Table 4.10. Moreover than contribution of material and utilities used to calculate environmental impacts of ethylene glycol is higher than contribution data used for dimethyl carbonate produced from CCU process, environmental impacts result in each impact also higher than environmental impacts result of dimethyl carbonate. However environmental impacts result in each impact of ethylene glycol is higher than dimethyl carbonate, environmental impact results from both LCSofT and SimaPro are in the same trend. There are some slightly different result between LCSofT and SimaPro in the same impacts which already discussed in environmental impacts result of dimethyl carbonate, such as freshwater ecotoxicity and human toxicity calculated from LCSofT are smaller than SimaPro because smaller sets of emission factors from combustion fuel and fossil depletion impact calculated by LCSofT is larger than SimaPro due to set of consuming fossil fuel in LCSofT is higher than SimaPro. The rest environmental impacts of ethylene glycol produced by CCU process are in the same trend and there are slightly different, however the results are in the acceptable range.

Carbon footprint of dimethyl carbonate and ethylene glycol produced from CCU process are shown in Table 4.15 and Figure 4.4. Carbon footprint results show amount of kg carbon dioxide equivalent produced from each unit per 1 kg of dimethyl carbonate (DMC) and ethylene glycol (EG) respectively in column 3 and 4. Column T2 in this process has the highest carbon footprint, so this unit should be optimized or changed some condition in order to decrease amount of utilities used in this unit. Not only column T2 should be optimized but also others columns, reactors and heat exchangers unit should be optimized or do heat integration in CCU process. Heat integration will help to decrease amount of utilities used for heat exchanger, so carbon footprint in heat exchanger can decrease more than the result as shown in Table 4.15 and Figure 4.4.

**Table 4.15** Carbon footprint (CO<sub>2</sub> eq.) of dimethyl carbonate and ethylene glycol produced from CCU process

Unit	Type of unit	Carbon Footprint (CO <sub>2</sub> eq.)	
		DMC	EG
P1	Pump	0.0207	0.0329
P2	Pump	0.0004	0.0007
P3	Pump	0.0058	0.0092
C2	Compressor	0.0282	0.0447
COMP_CH4	Compressor	3.3695	5.3513
COMP_CO2	Compressor	2.7514	4.3697
COMP_CO2_2	Compressor	1.3549	2.1519
COMP_EO	Compressor	0.4990	0.7925
COMP_H2O	Compressor	4.3745	6.9475
COMP_MEOH	Compressor	10.3972	16.5125
COMP_REC	Compressor	2.2339	3.5479
ECSYN	Reactor	0.4213	0.6691
EGSYN	Reactor	0.0341	0.0542
MEOHSYN	Reactor	7.51E-09	1.19E-08
COMREF	Reactor	14.9918	23.8094
F1	Flash	1.17E-09	1.86E-09
COOL_1	Heat Exchanger	2.2815	3.6234
COOL_2	Heat Exchanger	5.5982	8.8909
COOL_3	Heat Exchanger	0.6358	1.0098
COOL_5	Heat Exchanger	1.0150	1.6120
HEAT_1	Heat Exchanger	0.1745	0.2772
HEAT_2	Heat Exchanger	0.0775	0.1231
HEAT_H2O	Heat Exchanger	3.5439	5.6283
HX-1	Heat Exchanger	14.0914	22.3794
HX-2	Heat Exchanger	13.1266	20.8472
DIST_DMC_1condenser	Column-Condenser	5.7405	9.1169
DIST_DMC_1reboiler	Column-Reboiler	11.6089	18.4368
DIST_DMC_2condenser	Column-Condenser	3.4993	5.5575
DIST_DMC_2reboiler	Column-Reboiler	9.8655	15.6680
DIST_DMC_3condenser	Column-Condenser	0.0619	0.0984
DIST_DMC_3reboiler	Column-Reboiler	0.0622	0.0987
DIST_EC_1condenser	Column-Condenser	3.2907	5.2262
DIST_EC_1reboiler	Column-Reboiler	6.8574	10.8907
DIST_EGcondenser	Column-Condenser	0.0775	0.1230
DIST_EGreboiler	Column-Reboiler	0.2329	0.3699
DIST_MEOH_1condenser	Column-Condenser	0.2752	0.4371
DIST_MEOH_2condenser	Column-Condenser	2.7161	4.3137
DIST_MEOH_2reboiler	Column-Reboiler	5.5314	8.7847
T2condenser	Column-Condenser	28.7783	45.7046
T2reboiler	Column-Reboiler	70.3009	111.6495



**Figure 4.4** Carbon footprint of dimethyl carbonate (DMC) and ethylene glycol (EG) produced from CCU process.

Comparison of carbon footprint result calculated by previous and the latest version of LCSofT are shown in Table 4.16. For all compressor unit and DIST\_MEOH\_1condenser (this column is operated by using only condenser), carbon footprint results, calculated by previous version of LCSofT, are 0 kg CO<sub>2</sub> eq. (shown in third column with highlighted lines). even if these processes consume electricity, produced from natural gas at power plant, and chilled water, engine-driven chiller using natural gas respectively which these two processes of utilities always release CO<sub>2</sub> to environment. However, previous version of LCSofT cannot assess carbon footprint from some unit of CCU process, the latest version of LCSofT can assess carbon footprint (shown in last column of Table 4.16) and also all environmental impacts, produced from all unit in CCU process because compressors and column conditions are added into LCSofT already. To be exact that after compressor and more column conditions were added into LCSofT, the latest version of LCSofT can assess environmental impacts more precisely than previous version because LCSofT covers more equipment and techniques of industry:-

**Table 4.16** Carbon footprint (CO<sub>2</sub> eq.) of dimethyl carbonate produced from CCU process before and after adding compressor and column conditions

Unit	Type of unit	Carbon Footprint (CO <sub>2</sub> eq.)	
		Before	After
P1	Pump	0.0207	0.0207
P2	Pump	0.0004	0.0004
P3	Pump	0.0058	0.0058
C2	Compressor	0.00E+00	0.0282
COMP_CH4	Compressor	0.00E+00	3.3695
COMP_CO2	Compressor	0.00E+00	2.7514
COMP_CO2_2	Compressor	0.00E+00	1.3549
COMP_EO	Compressor	0.00E+00	0.499
COMP_H2O	Compressor	0.00E+00	4.3745
COMP_MEOH	Compressor	0.00E+00	10.3972
COMP_REC	Compressor	0.00E+00	2.2339
ECSYN	Reactor	0.4213	0.4213
EGSYN	Reactor	0.0341	0.0341
MEOHSYN	Reactor	7.51E-09	7.51E-09
COMREF	Reactor	14.9918	14.9918
F1	Flash	1.17E-09	1.17E-09
COOL_1	Heat Exchanger	2.2815	2.2815
COOL_2	Heat Exchanger	5.5982	5.5982
COOL_3	Heat Exchanger	0.6358	0.6358
COOL_5	Heat Exchanger	1.015	1.015
HEAT_1	Heat Exchanger	0.1745	0.1745
HEAT_2	Heat Exchanger	0.0775	0.0775
HEAT_H2O	Heat Exchanger	3.5439	3.5439
HX-1	Heat Exchanger	14.0914	14.0914
HX-2	Heat Exchanger	13.1266	13.1266
DIST_DMC_1condenser	Column-Condenser	5.7405	5.7405
DIST_DMC_1reboiler	Column-Reboiler	11.6089	11.6089
DIST_DMC_2condenser	Column-Condenser	3.4993	3.4993
DIST_DMC_2reboiler	Column-Reboiler	9.8655	9.8655
DIST_DMC_3condenser	Column-Condenser	0.0619	0.0619
DIST_DMC_3reboiler	Column-Reboiler	0.0622	0.0622
DIST_EC_1condenser	Column-Condenser	3.2907	3.2907
DIST_EC_1reboiler	Column-Reboiler	6.8574	6.8574
DIST_EGcondenser	Column-Condenser	0.0775	0.0775
DIST_EGreboiler	Column-Reboiler	0.2329	0.2329
DIST_MEOH_1condenser	Column-Condenser	0.00E+00	0.2752
DIST_MEOH_2condenser	Column-Condenser	2.7161	2.7161
DIST_MEOH_2reboiler	Column-Reboiler	5.5314	5.5314
T2condenser	Column-Condenser	28.7783	28.7783
T2reboiler	Column-Reboiler	70.3009	70.3009

**Table 4.17** Comparison of environmental impacts result per 1 kg of dimethyl carbonate from CCU process calculated by ReCiPe E, H, and I

Impact category	Unit	ReCiPe		
		E	H	I
<i>ReCiPe Midpoint</i>				
Climate Change	kg CO2 eq	2.28E+01	4.02E+01	8.03E+01
Ozone Depletion	kg CFC-11 eq	5.20E-12	5.20E-12	4.69E-12
Terrestrial Acidification	kg SO2 eq	1.24E-02	1.12E-02	1.02E-02
Freshwater Eutrophication	kg P eq	0.00E+00	0.00E+00	0.00E+00
Marine Eutrophication	kg N eq	3.28E-04	3.28E-04	3.20E-04
Human Toxicity	kg 1,4-DB eq	1.01E+02	3.45E-02	1.06E-02
Photochemical Oxidant Formation	kg NMVOC	1.86E-02	1.86E-02	1.82E-02
Particulate Matter Formation	kg PM10 eq	3.72E-03	3.72E-03	3.53E-03
Terrestrial Ecotoxicity	kg 1,4-DB eq	2.19E-05	4.04E-06	3.78E-06
Freshwater Ecotoxicity	kg 1,4-DB eq	3.82E-03	3.82E-03	3.61E-03
Marine Ecotoxicity	kg 1,4-DB eq	2.50E+01	9.91E-03	8.85E-03
Ionising Radiation	kBq U235 eq	0.00E+00	0.00E+00	0.00E+00
Agricultural Land Occupation	m2a	0.00E+00	0.00E+00	0.00E+00
Urban Land Occupation	m2a	0.00E+00	0.00E+00	0.00E+00
Natural Land Occupation	m2	0.00E+00	0.00E+00	0.00E+00
Water Depletion	m3	1.10E-03	1.10E-03	5.20E-04
Metal Depletion	kg Fe eq	0.00E+00	0.00E+00	0.00E+00
Fossil Depletion	kg oil eq	4.86E+00	4.86E+00	4.70E+00
<i>ReCiPe Endpoint</i>				
Ecosystem	species/yr	1.44E-05	4.37E-07	9.57E-05
Human Health	DALY	8.39E-03	1.17E-04	1.88E-06
Resources	\$	8.03E-01	8.03E-01	2.43E-01

Environmental impacts result based on 1 kg of dimethyl carbonate produced from CCU process by using ReCiPe E (long term), H (default), and I (short term) as LCIA methodology are shown in Table 4.17. With three different sublevels in ReCiPe methodology can help users to consider their case study or process in different perspective. For example environmental impacts result of CCU process calculated by three different sublevels of ReCiPe (E, H, and I), LCIA methodology, is shown in Table 4.17. For long term consideration, ReCiPe (E) is used as LCIA methodology to assess environmental impacts result and CO<sub>2</sub> is raw material of CCU process, so climate change impact result calculated by using ReCiPe (E) is less than climate change impact result calculated by using ReCiPe (H and I) because CO<sub>2</sub> is

consumed all the time during operation. For other environmental impacts result calculated from ReCiPe (E) are higher than other environmental impacts result calculated from ReCiPe (H and I) because there are cumulative of emission in environment. For short term consideration, environmental impacts result calculated by ReCiPe (I) is less than environmental impacts result calculated by ReCiPe (E and H) because this sublevel consider within a short period of time, less emission cumulative in environment. But climate change impact is higher than result calculated by ReCiPe (E and H) for CCU process because there is less CO<sub>2</sub> consumed in a short period of time. For default and consensus sublevel of ReCiPe is ReCiPe (H) which is based on scientific model. Environmental impacts result calculated by ReCiPe (H) is between result calculated by ReCiPe (E and I). By adding three different perspectives for calculation by ReCiPe (E, H, and I) can cover more purpose of environmental and process consideration from different users.

**Table 4.18** Water scarcity footprint of dimethyl carbonate from CCU process

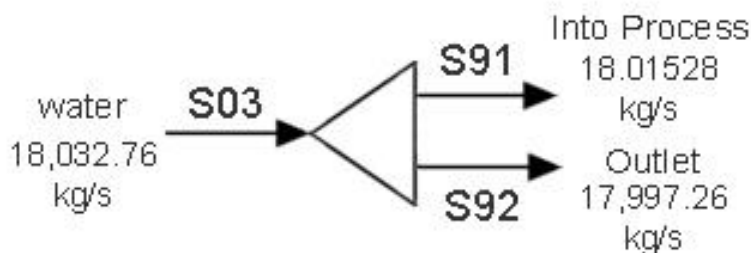
Month	Weather season in Denmark	Water Scarcity Footprint (m <sup>3</sup> /kg)
January	Winter	3.50788
February	Winter	3.77053
March	Winter	3.51443
April	Spring	4.50688
May	Spring	6.31094
June	Summer	9.9898
July	Summer	13.35375
August	Summer	15.56875
September	Autumn	15.22631
October	Autumn	11.66483
November	Autumn	8.11415
December	Winter	4.63876

Normally water is used in every process and total water consumption used to produce dimethyl carbonate (product) and ethylene glycol (co product) from CCU process is 18034.76 kg/s, this amount of water is total amount of water used in CCU process without allocation for dimethyl carbonate or ethylene glycol and difference between water input and output is not considered (water scarcity footprint

is considered only water input to the process). For this case water scarcity footprint in LCSoft consider amount of water used per 1 kg of pure dimethyl carbonate by using the amount of water from simulation result. In order to do a water scarcity footprint, some conditions are required to select, such as location of plant, purpose of using water, and etc. There are assumptions for calculate water scarcity footprint of this process. Assumptions are water is used for non-agricultural and this process is located in Denmark. LCSoft calculates the water scarcity footprint by based on input data and assumptions. In calculation of water scarcity footprint there are some different characterization factors in each country and month. Water scarcity footprint result of dimethyl carbonate produced from CCU process in each month is shown in Table 4.18.

From Table 4.18 show the different season throughout the year in Denmark and water scarcity footprint results in each month. This results show amount of water needed to regenerate or compensate to meet country's demand. As a result of using water as a part of raw material of CCU process. In order to produce 1 kg of dimethyl carbonate from CCU process this country will needed 15.56875 cubic meter of water per 1 kg of dimethyl carbonate, produced in summer.

Water scarcity footprint result of CCU process located in Denmark is different in each month because of season, shown in Table 4.18. The result value is very high during July to September because in that period is the summer season in Denmark, so there is water in the same natural source less than others season. The water scarcity footprint values will continuously decreasing from October until March because August is the last month of summer season. Autumn and winter will start in September and December respectively. There is a lot of rain and snow in winter, so water scarcity footprint in this period is continuously decreasing until spring season which comes in April and change to summer in June again. However, amount of water fed into this process is too high because there is 18,034.76 kg/s of water fed to splitter unit in this process, but just only 18.01528 kg/s from 18,034.76 kg/s is fed into others part of process and the rest of water are fed out from this process as shown in Figure 4.5.



**Figure 4.5** Water flow rate at splitter in CCU process.

For more proper and precisely in water scarcity footprint calculation of CCU process, there are more new assumptions for calculation of water scarcity footprint in this case study. Only amount of water fed into process is considered and except water from stream S92 as shown in Figure 4.5. Stream S92 is neglected for water scarcity footprint calculation because water from stream S03 passes through the splitter and only 18.01528 kg/s (stream S91) from 18,032.76 kg/s (stream S03) flows into the others part of process. Amount of water used in this process is allocated before calculate the water scarcity footprint. Amount of water is allocated by using molar flow rate of dimethyl carbonate (product) and ethylene glycol (co product) same as the allocation of material and utilities. There is not water treatment unit in CCU process and others assumptions for water scarcity footprint calculation are the same as mentioned before. The amount of water used in each stream which is fed into process with and without allocation is shown in Table 4.19

**Table 4.19** Amount of water used for CCU process with and without allocation

Stream	Water flow rate (kg/s)		
	Total amount of water	With allocation	
		DMC	EG
S01	6.50	2.51	3.99
S91	18.02	6.96	11.05
Water	12.61	4.87	7.74
Water_2	0.36	0.14	0.22
Total	37.49	14.49	23.01



**Table 4.20** Water scarcity footprint result with and without allocation

Month	Water Scarcity Footprint (m <sup>3</sup> /kg)		
	Without allocation	DMC	EG
January	0.0189	0.0073	0.0106
February	0.0203	0.0078	0.0114
March	0.0189	0.0073	0.0106
April	0.0243	0.0094	0.0136
May	0.0340	0.0131	0.0190
June	0.0538	0.0208	0.0301
July	0.0719	0.0278	0.0403
August	0.0838	0.0324	0.0470
September	0.0820	0.0317	0.0460
October	0.0628	0.0243	0.0352
November	0.0437	0.0169	0.0245
December	0.0250	0.0096	0.0140

Table 4.20 shows water scarcity footprint result by using the amount of water input with and without allocation for dimethyl carbonate and ethylene glycol as shown in Table 4.19. The water scarcity footprint result without allocation is based on 1 kg of dimethyl carbonate (product) and others result with allocation are based on 1 kg of dimethyl carbonate and ethylene glycol for product and co product respectively. All results in Table 4.20 are shown in the same trend of result from Table 4.18 which scarcity of water also depends on the period of time (different season in each country). The water scarcity footprint with new condition is more suitable than the results in Table 4.18 because result from previous condition just only 1 kg of product produced in January at Denmark, so this country will need 3.50788 m<sup>3</sup> to compensate because previous condition 18032.76 kg/s of water is used for water scarcity footprint calculation instead of 18.01528 kg/s which is the amount of water used in the whole part of process. For this result can help the company and government in each country make a good decision to establish or approve the future project which will give many benefits back to environmental especially about quality and quantity of water resource in every country and our planet. Moreover, if there is water pretreatment unit to treat water to meet the specification of people using or legal in each country before release to environmental, user can consider only amount of water disappear from the process (amount of water input minus output) as water

consumption instead of all of water input to the process for water scarcity footprint calculation. With this condition water scarcity footprint in each month and process will decrease more than results in Table 4.20.

CCU process, case study in this thesis, is under development by Ph.D. student at Technical University of Denmark (DTU). Dimethyl carbonate produced from CCU process consumes 9.31 kg of water per 1 kg of dimethyl carbonate. To prove the suitability amount of water consumption in this process, ratio of water consumption per 1 kg of product is compared with another petrochemical product. Sodium carbonate produced from trona in fluidized bed reactor, which plant is located in Italy, consumes 14.58 kg of water per 1 kg of sodium carbonate (Bonaventura et al., 2017). Water consumption to produce sodium carbonate is higher than water consumption for dimethyl carbonate because reactions, technologies and techniques between two processes are slightly different that mean amount of water consumed in CCU process is suitable for petrochemical process.

Ecological footprint result of this plant which is located in Denmark is shown in different purpose of land used; built up land, carbon, cropland, fishing grounds, forest products, and grazing land, and different unit; biocapacity (gha), ecological footprint (gha per person, gha, and number of earths) as shown in Table 4.21.

**Table 4.21** Ecological footprint result in Denmark

	Biocapacity (gha)	Ecological Footprint (gha per person)	Ecological Footprint (gha)	Ecological Footprint Number of Earths)
Built up Land	1,291,929.36	0.2297	1,291,929.36	0.1347
Carbon	0.0000	3.1130	17,508,215.40	1.8255
Cropland	12,311,400.81	1.1304	6,357,629.61	0.6629
Fishing Grounds	10,170,337.75	0.2414	1,357,972.68	0.1416
Forest Products	1,907,354.39	0.8932	5,023,717.20	0.5238
Grazing Land	43,690.97	0.5007	2,815,810.46	0.2936
Total	25,724,713.28	6.1084	34,355,274.70	3.5820

Results from Table 4.21 show the collected data about biocapacity and ecological footprint in Denmark in 2013. The last row from Table 4.21, total of biocapacity is less than ecological footprint, that mean human's demand on resource is more than supply of natural resource can regenerate to support human's demand on nature. For cropland biocapacity is more than ecological footprint, so Denmark government can promote their people to do or invest more in agricultural instead of fishing, deforestation, and animal farming because all of this kind of business have biocapacity less than ecological footprint. However biocapacity and ecological footprint is only one factor to assess about land used in each country, because there are different of area site, geography, weather, amount of people, tradition, and etc. in each country as shown in Table 4.22. Ecological footprint can be used as a preliminary assessment before make a decision or approve a new project in the future.

**Table 4.22** Area and population in Denmark

Country	Population (million people)	Area (sq. km)
Denmark	5.615	43,560

Furthermore water scarcity footprint and ecological footprint are provided in LCSoft, they also needed an update data or method used in calculation because there are many factors which have an effect on results for example situation of weather change every year, higher population, high human demand, resource available, and etc.

## **CHAPTER V**

### **CONCLUSIONS AND RECOMMENDATIONS**

#### **5.1 Conclusions**

The growth of industries and increasing of population and human's demand on natural resource in the past decades, Life cycle assessment (LCA) technique become the most popular tool to assess environmental impact caused by human's demand. There is much LCA software available, but LCSOFT has been developed to do LCA calculation in a concept of user friendly and has ability to integrate with others simulation software. In order to cover wider range of application, there are many parts of LCSOFT which were developed. More column conditions in industry are added into LCSOFT for more correctly in calculation. ReCiPe midpoint and endpoint with three different perspectives, egalitarian, individualist, and hierachist were added into LCIA methodologies selection. Water scarcity footprint and ecological footprint were added into LCSOFT as an optional function in interpretation step. Finally environmental results, calculated from LCSOFT, were validated with commercial LCA software, SimaPro version 8.3., through two case studies, bioethanol from cassava rhizome (biochemical process) and dimethyl carbonate from carbon dioxide capture (CCU) (petrochemical process). With new condition, LCIA methodologies, footprint interpretation, and validation result show that LCSOFT has an ability to evaluate the environmental impacts from bioethanol and petrochemical process. Moreover LCSOFT has a wider range of application used than previous version with new condition, methodologies and interpretation choices, added into software. Therefore LCSOFT becomes as friendly, reliable and efficient software for LCA calculation.

#### **5.2 Recommendations**

However LCSOFT was developed and added many conditions and new features, the software should be developed and improved as shown in the following recommendations.

### 5.2.1 LCI Database

In order to cover wider range of application used, more LCI databases should be added into LCSofT. With wider range of database user can evaluate environmental impact more reliable and precisely.

### 5.2.2 LCIA Methodologies

More LCIA methodologies should be added into LCIA method selection, in order to cover widely of user from different country and continent because in some country they have their own LCIA method which is more precisely in calculation than others method for that country.

### 5.2.3 Water Footprint and Water Scarcity Footprint

Water scarcity footprint was already added into the latest version of LCSofT, but in the near future new water footprint or water scarcity footprint method will be updated with more correct data and up-to-date with human's consumption on water and water available in that time. Water scarcity footprint in LCSofT should be updated or added water footprint with a consensus model in that time.

### 5.2.4 Ecological Footprint

Ecological footprint was provided in LCSofT, but they also needed an update data or changed the method used in calculation because there are many factors which have an effect to the results for examples higher in population, higher human's demand, decreasing of natural source available, new technologies in industry or agriculture, and etc.

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# APPENDICES

## Appendix A Bioethanol from Cassava Rhizome Process Details

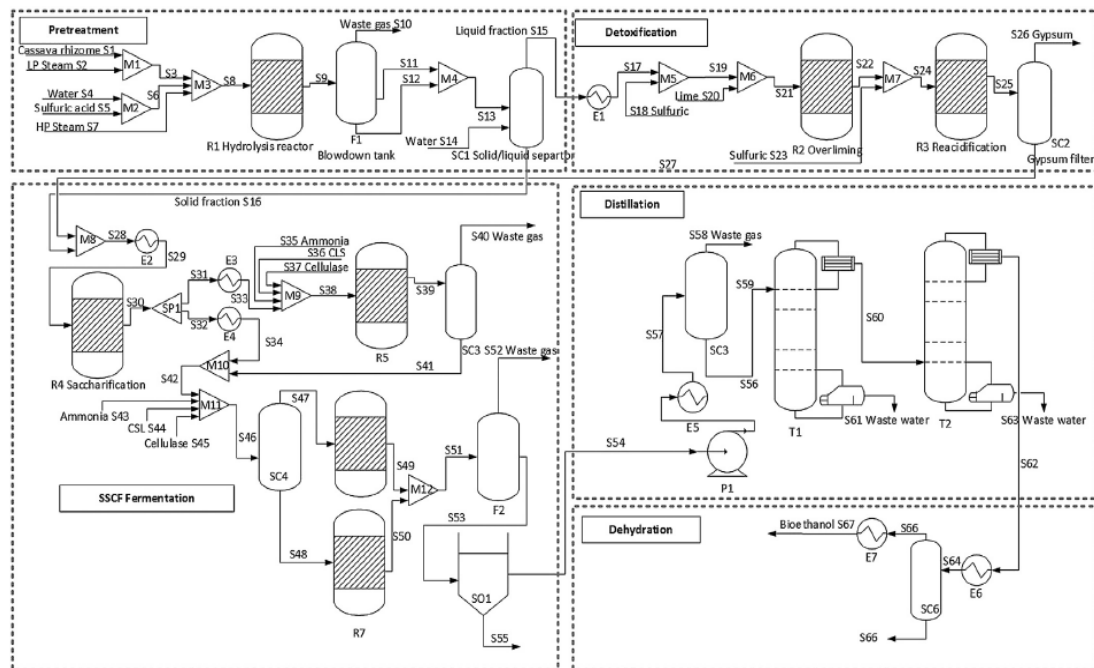


Figure A1 Bioethanol from cassava rhizome process flowsheet.

**Table A1** Stream table of bioethanol from cassava rhizome process

Stream Name		S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15
Stream Description																
Stream Phase		Mixed	Vapor	Mixed	Liquid	Liquid	Liquid	Vapor	Mixed	Mixed	Vapor	Liquid	Solid	Mixed	Liquid	Mixed
Temperature	C	30.000	160.000	100.018	25.000	25.000	25.000	268.000	188.002	190.000	103.854	103.854	103.854	103.854	25.000	62.663
Pressure	ATM	1.000	6.000	1.000	1.000	1.000	1.000	13.000	12.100	12.100	1.000	1.000	1.000	1.000	1.000	1.000
Total Molecular Weight		103.896	18.015	84.688	18.015	98.079	18.308	18.015	38.223	40.920	18.725	35.367	94.665	47.174	18.015	23.111
<b>Total Weight Comp. Rates</b>	kg/hr															
Cellulose		4680.59	0.00	4680.59	0.00	0.00	0.00	0.00	4680.59	4320.19	0.00	0.00	4320.19	4320.19	0.00	21.60
Hemicellulose		6674.09	0.00	6674.09	0.00	0.00	0.00	0.00	6674.09	333.70	0.00	0.00	333.70	333.70	0.00	1.67
Lignin		3653.45	0.00	3653.45	0.00	0.00	0.00	0.00	3653.45	3653.45	0.00	0.00	3653.45	3653.45	0.00	18.27
Glucose		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	364.05	0.00	364.05	0.00	364.05	0.00	287.60
Xylose		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6825.73	0.00	6825.73	0.00	6825.73	0.00	4436.73
Cellulose		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	34.58	0.00	34.58	0.00	34.58	0.00	27.32
Ethanol		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Water		129.52	785.09	914.61	4972.11	0.00	4972.11	3153.38	9040.11	8273.83	2371.59	5902.24	0.00	5902.24	12898.25	14852.38
Sulfuric Acid		0.00	0.00	0.00	0.00	99.44	99.44	0.00	99.44	99.44	0.00	99.44	0.00	99.44	0.00	78.56
Furfural		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	242.70	115.98	126.71	0.00	126.71	0.00	100.10
Ammonia		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Oxygen		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Carbon Dioxide		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Glycerol		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Succinic Acid		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Lactic Acid		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HMF		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Xylitol		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Acetic Acid		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CornSteep Liquor		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ZM		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cellulase		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Lime		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CASO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ash		578.25	0.00	578.25	0.00	0.00	0.00	0.00	578.25	578.25	0.00	0.00	578.25	578.25	0.00	0.00

**Table A1** Stream table of bioethanol from cassava rhizome process (cont'd)

Stream Name		S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26	S27	S28	S29	S30
Stream Description																
Stream Phase		Mixed	Mixed	Liquid	Mixed	Solid	Mixed	Mixed	Liquid	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed
Temperature	C	62.663	50.000	25.000	49.941	25.000	49.861	49.861	25.000	49.836	49.836	49.836	49.836	54.135	65.000	65.000
Pressure	ATM	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Total Molecular Weight		46.462	23.111	98.079	23.210	74.093	23.353	23.301	98.079	23.342	23.329	137.765	22.980	29.476	29.476	30.087
<b>Total Weight Comp. Rates</b>	kg/hr															
Cellulose		4298.59	21.60	0.00	21.60	0.00	21.60	21.60	0.00	21.60	21.60	21.60	0.00	4298.59	4298.59	378.28
Hemicellulose		332.04	1.67	0.00	1.67	0.00	1.67	1.67	0.00	1.67	1.67	1.67	0.00	332.04	332.04	332.04
Lignin		3635.18	18.27	0.00	18.27	0.00	18.27	18.27	0.00	18.27	18.27	0.00	18.27	3653.45	3653.45	3653.45
Glucose		76.45	287.60	0.00	287.60	0.00	287.60	287.60	0.00	287.60	287.60	0.58	287.02	363.47	363.47	4698.47
Xylose		2389.01	4436.73	0.00	4436.73	0.00	4436.73	4436.73	0.00	4436.73	4436.73	8.87	4427.85	6816.86	6816.86	6816.86
Cellobiose		7.26	27.32	0.00	27.32	0.00	27.32	27.32	0.00	27.32	27.32	0.00	27.32	34.58	34.58	54.45
Ethanol		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Water		3948.10	14852.38	0.00	14852.38	0.00	14852.38	14922.47	0.00	14922.47	14939.62	0.00	14939.62	18887.72	18887.72	18453.19
Sulfuric Acid		20.88	78.56	112.24	190.79	0.00	190.79	0.00	46.66	46.66	0.00	0.00	0.00	20.88	20.88	20.88
Furfural		26.61	100.10	0.00	100.10	0.00	100.10	100.10	0.00	100.10	100.10	0.20	99.90	126.51	126.51	126.51
Ammonia		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Oxygen		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Carbon Dioxide		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Glycerol		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Succinic Acid		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Lactic Acid		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HMF		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Xylitol		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Acetic Acid		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CornSteep Liquor		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ZM		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cellulase		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Lime		0.00	0.00	0.00	0.00	179.42	179.42	35.28	0.00	35.28	0.03	0.03	0.00	0.00	0.00	0.00
CASO4		0.00	0.00	0.00	0.00	0.00	0.00	264.84	0.00	264.84	329.61	329.61	0.00	0.00	0.00	0.00
Ash		578.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	578.25	578.25	578.25

**Table A1** Stream table of bioethanol from cassava rhizome process (cont'd)

Stream Name		S31	S32	S33	S34	S35	S36	S37	S38	S39	S40	S41	S42	S43	S44	S45
Stream Description																
Stream Phase		Mixed	Mixed	Mixed	Mixed	Vapor	Liquid	Mixed	Mixed	Mixed	Vapor	Mixed	Mixed	Vapor	Liquid	Solid
Temperature	C	65.000	65.000	41.562	40.858	25.000	25.000	25.000	41.000	41.000	42.531	42.531	41.033	25.000	25.000	25.000
Pressure	ATM	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Total Molecular Weight		30.087	30.087	30.087	30.087	17.031	18.015	18.090	29.546	26.166	43.990	24.607	29.497	17.031	18.015	22.840
<b>Total Weight Comp. Rates</b>	kg/hr															
Cellulose		37.83	340.45	37.83	340.45	0.00	0.00	0.00	37.83	37.83	0.00	37.83	378.28	0.00	0.00	0.00
Hemicellulose		33.20	298.83	33.20	298.83	0.00	0.00	0.00	33.20	33.20	0.00	33.20	332.04	0.00	0.00	0.00
Lignin		365.34	3288.10	365.34	3288.10	0.00	0.00	0.00	365.34	365.34	0.00	365.34	3653.45	0.00	0.00	0.00
Glucose		469.85	4228.63	469.85	4228.63	0.00	0.00	0.00	469.85	43.90	0.00	43.90	4272.52	0.00	0.00	0.00
Xylose		681.69	6135.17	681.69	6135.17	0.00	0.00	0.00	681.69	121.40	0.00	121.40	6256.57	0.00	0.00	0.00
Cellobiose		5.44	49.00	5.44	49.00	0.00	0.00	0.00	5.44	5.44	0.00	5.44	54.45	0.00	0.00	0.00
Ethanol		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	495.17	37.14	458.03	458.03	0.00	0.00	0.00
Water		1845.32	16607.87	1845.32	16607.87	0.00	0.00	37.74	1883.06	1883.99	0.94	1883.04	18490.92	0.00	0.00	0.00
Sulfuric Acid		2.09	18.79	2.09	18.79	0.00	0.00	0.00	2.09	2.09	0.00	2.09	20.88	0.00	0.00	0.00
Furfural		12.65	113.86	12.65	113.86	0.00	0.00	0.00	12.65	12.65	0.00	12.65	126.51	0.00	0.00	0.00
Ammonia		0.00	0.00	0.00	0.00	0.83	0.00	0.00	0.83	0.00	0.00	0.00	0.00	2.48	0.00	0.00
Oxygen		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.38	1.38	0.00	0.00	0.00	0.00	0.00
Carbon Dioxide		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	472.36	448.74	23.62	23.62	0.00	0.00	0.00
Glycerol		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.59	0.00	0.59	0.59	0.00	0.00	0.00
Succinic Acid		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.82	0.00	1.82	1.82	0.00	0.00	0.00
Lactic Acid		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.33	0.00	0.33	0.33	0.00	0.00	0.00
HMF		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Xylitol		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.08	0.00	6.08	6.08	0.00	0.00	0.00
Acetic Acid		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.40	0.00	2.40	2.40	0.00	0.00	0.00
CornSteep Liquor		0.00	0.00	0.00	0.00	0.00	59.69	0.00	59.69	59.69	0.00	59.69	59.69	0.00	87.78	0.00
ZM		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.01	0.00	6.01	6.01	0.00	0.00	0.00
Cellulase		0.00	0.00	0.00	0.00	0.00	0.00	0.76	0.76	0.76	0.00	0.76	0.76	0.00	0.00	7.57
Lime		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CASO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ash		57.83	520.43	57.83	520.43	0.00	0.00	0.00	57.83	57.83	0.00	57.83	578.25	0.00	0.00	0.00

**Table A1** Stream table of bioethanol from cassava rhizome process (cont'd)

Stream Name		S46	S47	S48	S49	S50	S51	S52	S53	S54	S55	S56	S57	S58	S59	S60
Stream Description																
Stream Phase		Mixed	Mixed	Liquid	Mixed	Liquid	Mixed	Vapor	Mixed	Liquid	Solid	Liquid	Liquid	Vapor	Liquid	Vapor
Temperature	C	41.000	41.000	41.000	41.000	41.000	41.021	41.021	41.021	41.021	41.021	41.240	100.510	100.000	100.000	93.831
Pressure	ATM	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	4.760	4.760	4.760	4.760	1.770
Total Molecular Weight		29.446	29.227	161.023	25.907	90.079	26.075	42.297	24.681	22.152	67.371	22.152	22.152	42.462	21.890	38.742
<b>Total Weight Comp. Rates</b>	kg/hr															
Cellulose		378.28	378.28	0.00	37.37	0.00	37.37	0.00	37.37	0.00	37.37	0.00	0.00	0.00	0.00	0.00
Hemicellulose		332.04	332.04	0.00	332.04	0.00	332.04	0.00	332.04	0.00	332.04	0.00	0.00	0.00	0.00	0.00
Lignin		3653.45	3653.45	0.00	3653.45	0.00	3653.45	0.00	3653.45	0.00	3653.45	0.00	0.00	0.00	0.00	0.00
Glucose		4272.52	4144.35	128.18	218.43	0.00	218.43	0.00	218.43	218.43	0.00	218.43	218.43	0.00	218.43	0.00
Xylose		6256.57	6068.87	187.70	828.31	0.00	828.31	0.00	828.31	828.31	0.00	828.31	828.31	0.00	828.31	0.00
Cellobiose		54.45	54.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethanol		458.03	458.03	0.00	5321.67	0.00	5321.67	258.60	5063.08	5063.08	0.00	5063.08	5063.08	15.19	5047.89	4987.13
Water		18490.92	18490.92	0.00	18449.79	0.00	18449.79	131.71	18318.08	18318.08	0.00	18318.08	18318.08	16.49	18301.59	689.61
Sulfuric Acid		20.88	20.88	0.00	20.88	0.00	20.88	0.00	20.88	20.88	0.00	20.88	20.88	0.00	20.88	0.00
Furfural		126.51	126.51	0.00	126.51	0.00	126.51	2.19	124.32	124.32	0.00	124.32	124.32	0.74	123.58	0.36
Ammonia		2.48	2.48	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Oxygen		0.00	0.00	0.00	7.76	0.00	7.76	7.65	0.11	0.11	0.00	0.11	0.11	0.11	0.00	0.00
Carbon Dioxide		23.62	23.62	0.00	4665.47	0.00	4665.47	4068.94	596.53	596.53	0.00	596.53	596.53	596.53	0.00	0.00
Glycerol		0.59	0.59	0.00	4.24	0.00	4.24	0.00	4.24	4.24	0.00	4.24	4.24	0.00	4.24	0.00
Succinic Acid		1.82	1.82	0.00	13.60	0.00	13.60	0.00	13.60	13.60	0.00	13.60	13.60	0.00	13.60	0.00
Lactic Acid		0.33	0.33	0.00	2.43	315.87	318.30	0.00	318.30	318.30	0.00	318.30	318.30	0.00	318.30	0.00
HMF		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Xylitol		6.08	6.08	0.00	47.59	0.00	47.59	0.00	47.59	47.59	0.00	47.59	47.59	0.00	47.59	0.00
Acetic Acid		2.40	2.40	0.00	17.51	0.00	17.51	0.15	17.36	17.36	0.00	17.36	17.36	0.01	17.36	0.01
CornSteep Liquor		147.47	147.47	0.00	147.47	0.00	147.47	0.57	146.91	146.91	0.00	146.91	146.91	0.13	146.78	0.04
ZM		6.01	6.01	0.00	23.96	0.00	23.96	0.00	23.96	0.00	23.96	0.00	0.00	0.00	0.00	0.00
Cellulase		8.32	8.32	0.00	8.32	0.00	8.32	0.00	8.32	0.00	8.32	0.00	0.00	0.00	0.00	0.00
Lime		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CASO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ash		578.25	578.25	0.00	578.25	0.00	578.25	0.00	578.25	0.00	578.25	0.00	0.00	0.00	0.00	0.00

**Table A1** Stream table of bioethanol from cassava rhizome process (cont'd)

Stream Name		S61	S62	S63	S64	S65	S66	S67
Stream Description								
Stream Phase		Liquid	Liquid	Liquid	Vapor	Vapor	Vapor	Liquid
Temperature	C	116.676	93.343	109.986	100.000	100.018	100.018	40.000
Pressure	ATM	1.770	1.770	1.770	1.770	1.000	1.000	1.000
Total Molecular Weight		19.419	42.121	18.746	42.121	46.033	18.015	46.033
<b>Total Weight Comp. Rates</b>	kg/hr							
Cellulose		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Hemicellulose		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Lignin		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Glucose		218.43	0.00	0.00	0.00	0.00	0.00	0.00
Xylose		828.31	0.00	0.00	0.00	0.00	0.00	0.00
Cellobiose		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethanol		60.76	4962.20	24.93	4962.20	4962.20	0.00	4962.20
Water		17611.99	317.86	371.75	317.86	2.48	315.38	2.48
Sulfuric Acid		20.88	0.00	0.00	0.00	0.00	0.00	0.00
Furfural		123.23	0.00	0.36	0.00	0.00	0.00	0.00
Ammonia		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Oxygen		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Carbon Dioxide		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Glycerol		4.24	0.00	0.00	0.00	0.00	0.00	0.00
Succinic Acid		13.60	0.00	0.00	0.00	0.00	0.00	0.00
Lactic Acid		318.30	0.00	0.00	0.00	0.00	0.00	0.00
HMF		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Xylitol		47.59	0.00	0.00	0.00	0.00	0.00	0.00
Acetic Acid		17.34	0.00	0.01	0.00	0.00	0.00	0.00
CornSteep Liquor		146.74	0.00	0.04	0.00	0.00	0.00	0.00
ZM		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cellulase		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Lime		0.00	0.00	0.00	0.00	0.00	0.00	0.00
CASO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ash		0.00	0.00	0.00	0.00	0.00	0.00	0.00

**Table A2** Equipment table of bioethanol from cassava rhizome process

<b>Pump</b>		
<b>Pump Name</b>		<b>P1</b>
Work	KWH	5.698

<b>Reactor</b>								
<b>ConReactor Name</b>		<b>R1</b>	<b>R2</b>	<b>R3</b>	<b>R4</b>	<b>R5</b>	<b>R6</b>	<b>R7</b>
Temperature	C	190	50	50	65	41	41	41
Pressure	ATM	12.100	1.000	1.000	1.000	1.000	1.000	1.000
Duty	MJ/HR	0.000	-399.600	-97.700	1613.200	-843.300	-8214.400	-322.900
Heat Of Reaction	MJ/HR	-1.29	-0.38	-0.09	-0.88	-0.01	-0.38	0.09
Product Enthalpy	KJ/KG	-227.73	1309.97	1335.91	821.19	-36.54	-272.51	8.34
Feed Enthalpy	KJ/KG	-4142.82	1205.76	1310.42	-1562.67	19.70	39.69	31.74
$\Delta$ Enthalpy	KJ/KG	3915.09	104.21	25.49	2383.86	-56.24	-312.20	-23.39
	GJ/KG	3.92	0.10	0.03	2.38	-0.06	-0.31	-0.02

<b>Flash</b>			
<b>Flash Name</b>		<b>F1</b>	<b>F2</b>
Temperature	C	103.854	41.021
Pressure	ATM	1.00	1.00
DP	ATM	11.10	0.00
Duty	MJ/HR	0.00	0.00



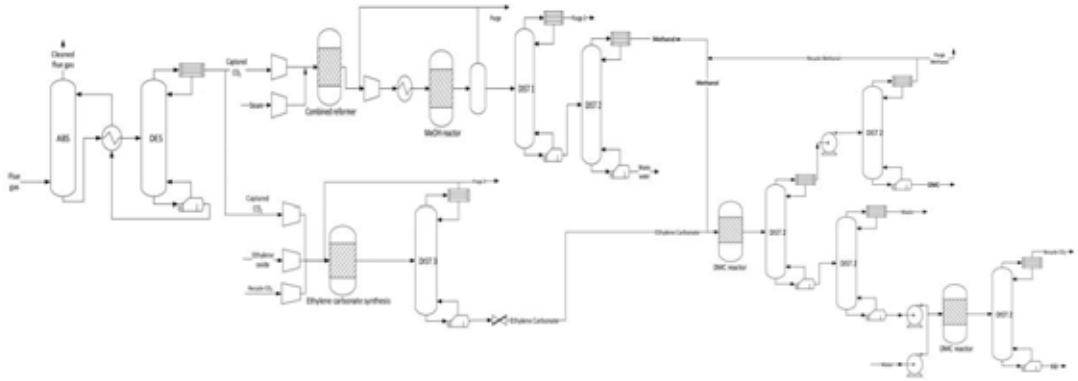
**Table A2** Equipment table of bioethanol from cassava rhizome process (cont'd)

<b>Stream Calculator</b>							
<b>Stream Calculator Name</b>		<b>SC1</b>	<b>SC2</b>	<b>SC3</b>	<b>SC4</b>	<b>SC5</b>	<b>SC6</b>
Duty	MJ/HR	0.00	0.00	0.00	0.00	0.00	0.00
Overhead Product Temperature	C	62.66	49.84	42.53	41.00	100.00	100.02
Bottoms Product Temperature	C	62.66	49.84	42.53	41.00	100.00	100.02

<b>Heat Exchanger</b>								
<b>Hx Name</b>		<b>E1</b>	<b>E2</b>	<b>E3</b>	<b>E4</b>	<b>E5</b>	<b>E6</b>	<b>E7</b>
Duty	MJ/HR	859.30	1113.00	235.20	2180.00	5678.50	4804.00	4840.40

<b>Column</b>			
<b>Column Name</b>		<b>T1</b>	<b>T2</b>
Condenser Duty	MJ/HR	-18089.20	-19971.20
Reboiler Duty	MJ/HR	24889.60	14371.40
Column Total Molar Feed	KG-MOL/DAY	27507.28	3517.02
Column Total Wt. Feed	KG/DAY	602124.67	136253.11
Column Condenser Pres	ATM	1.77	1.77
Column Condenser Temp	C	93.83	93.34
Column Reflux Rate	KG-MOL/DAY	0.00	9628.49
Column Reflux Ratio		3.20	3.20

## Appendix B Dimethyl Carbonate and Ethylene Glycol from Carbon Dioxide Capture and Utilization (CCU) Process



**Figure B1** Dimethyl carbonate and ethylene glycol from carbon dioxide capture and utilization process flowsheet

**Table B1** Stream table of dimethyl carbonate from CCU process without allocation

Stream Name		CO2	CO2PURGE	CO2_2	DMC	EC	EG	EO	MEOH	PURGE	PURGE2	PURGE3
Stream Description												
Stream Phase		Vapor	Vapor	Vapor	Liquid	Liquid	Liquid	Vapor	Liquid	Vapor	Vapor	Vapor
Temperature	K	312.7119591	312.7119591	312.7119591	492.876141	614.2843	595.4784	298.15	403.4818876	333.15	389.5933	247.6273
Pressure	bar	1.21	1.21	1.21	20	10	25	1	10	59	10.5	9
Total Molecular Weight		42.42437109	42.42437109	42.42437109	89.4846824	87.6227	61.93991	44.05316	32.07548119	22.47725322	33.63472	44.01038
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.038	0.008	0.009	0.000	0.000	0.000	0.000	0.000	0.038	0.000	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		24.773	5.168	6.193	0.000	0.000	0.014	0.000	0.000	6.952	0.744	3.756
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.644	0.134	0.161	0.001	0.000	0.004	0.000	0.000	0.046	0.066	0.000
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	11.647	0.111	0.000
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.487	0.002	0.000
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.166	0.037	0.000
METHANOL		0.000	0.000	0.000	0.013	0.000	0.000	0.000	0.000	0.367	0.615	0.000
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.033	0.000	3.304	0.000	0.000	0.000	0.051
EG		0.000	0.000	0.000	0.000	0.000	4.411	0.000	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	4.031	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		0.000	0.000	0.000	0.000	6.438	0.018	0.000	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B1** Stream table of dimethyl carbonate from CCU process without allocation (cont'd)

Stream Name		PURGEMEOH	PURGE_CO2_2	REC_CO2	REC_MEOH	S01	S01_R1	S01_R2	S02	S03	S1	S10
Stream Description												
Stream Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Liquid	Liquid	Liquid	Vapor
Temperature	K	436.5875563	262.1817386	262.181739	436.5875563	320.4934	320.49339	320.4933941	319.15	320	417.01	1174.811
Pressure	bar	19	24.5	24.5	19	1.567	1.567	1.567	1.013	1.013	10.5	25
Total Molecular Weight		33.08009793	44.00979474	44.0097947	33.08009793	29.83503	29.835026	29.83502582	61.08372	18.01528	24.688	24.64763
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.000	0.000	0.000	113.399	113.399	113.399	0.000	0.000	0.000	0.038
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.059	0.087	0.780	0.168	36.137	36.137	36.137	0.000	0.000	0.059	24.773
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.000	0.000	0.000	0.000	6.501	6.501	6.501	0.000	18015.28	9.974	13.255
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	61080.00	0.000	0.000	0.000
CO		0.001	0.000	0.000	0.004	0.000	0.000	0.000	0.000	0.000	0.001	0.000
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METHANE		0.001	0.000	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.001	11.230
METHANOL		9.120	0.000	0.000	26.056	0.000	0.000	0.000	0.000	0.000	15.984	0.000
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.033	0.000	0.000	0.093	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DMCARB		0.433	0.000	0.000	1.237	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B1** Stream table of dimethyl carbonate from CCU process without allocation (cont'd)

Stream Name		S11	S12	S13	S14	S15	S16	S17	S18	S19	S2	S20
Stream Description												
Stream Phase		Vapor	Liquid	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Mixed	Vapor
Temperature	K	620.8438467	342.2768525	631.6311723	885.9905	699.2349	1188.2	729.2349	756.3417891	513.15	384	816.0595
Pressure	bar	25	1.58	25	25	25	25	24	60	60	1.58	59
Total Molecular Weight		16.04276085	30.8203054	42.42437109	18.0152798	24.64763	24.64792	15.77359	18.21748263	18.21748263	30.82031	23.21638
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.055	0.038	0.000	0.038	0.000	0.000	0.108	0.108	0.055	0.108
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.000	70.852	24.773	0.000	24.773	0.000	0.000	23.566	23.566	70.852	20.665
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.000	376.123	0.644	0.000	13.255	0.000	0.000	8.983	8.983	376.123	10.170
MEA		0.000	496.729	0.000	0.000	0.000	0.000	0.000	0.000	0.000	496.729	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	46.373	46.373	0.000	33.389
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	3.659	3.659	0.000	1.392
METHANE		11.230	0.000	0.000	0.000	11.230	0.000	0.000	6.226	6.226	0.000	6.226
METHANOL		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.681	0.681	0.000	17.647
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B1** Stream table of dimethyl carbonate from CCU process without allocation (cont'd)

Stream Name		S21	S22	S23	S24	S25	S26	S27	S28	S29	S3	S30
Stream Description												
Stream Phase		Liquid	Vapor	Vapor	Mixed	Mixed	Vapor	Vapor	Vapor	Vapor	Vapor	Liquid
Temperature	K	333.15	333.15	961.257771	333.568983	333.15	579.95063	566.8089	333.15	733.6021	318.58	405.2644
Pressure	bar	59	59	125	11	59	24	125	59	59	1.01	10
Total Molecular Weight		25.0688	22.4773	44.0098	25.0688	23.2164	18.2175	44.0135	22.4773	23.2164	27.3525	36.6843
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.108	0.000	0.000	0.108	0.108	0.000	0.070	0.108	113.343	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.803	19.862	6.193	0.803	20.665	23.566	40.778	12.910	20.665	0.006	0.168
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		10.040	0.130	0.000	10.040	10.170	8.983	0.000	0.085	10.170	5.316	0.002
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.142	0.000
CO		0.113	33.276	0.000	0.113	33.389	46.373	0.000	21.629	33.389	0.000	0.004
H2		0.002	1.390	0.000	0.002	1.392	3.659	0.000	0.904	1.392	0.000	0.000
METHANE		0.038	6.188	0.000	0.038	6.226	6.226	0.000	4.022	6.226	0.000	0.002
METHANOL		16.599	1.047	0.000	16.599	17.647	0.681	0.000	0.681	17.647	0.000	29.466
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.000	0.000	3.762	0.000	0.000	0.000	0.093
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.804
ETLNCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	6.438
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B1** Stream table of dimethyl carbonate from CCU process without allocation (cont'd)

Stream Name		S31	S32	S34	S35	S36	S37	S38	S39	S4	S40	S41
Stream Description												
Stream Phase		Vapor	Liquid	Vapor	Vapor	Mixed	Mixed	Vapor	Mixed	Liquid	Mixed	Liquid
Temperature	K	312.7223525	399.5043521	640.78791	383.15	383.15	320.9446	247.62726	417.540586	319.15	408.31	397.2447
Pressure	bar	1.21	1.778	125	125	125	10	9	10	1.778	10	9
Total Molecular Weight		42.42353127	30.47994507	44.0531616	44.0134593	47.440599	47.440599	44.010379	36.6843037	30.47995	38.705	35.98273
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.055	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		36.135	34.722	0.000	40.778	36.471	37.561	37.561	0.165	34.722	0.125	0.168
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.940	375.169	0.000	0.000	0.000	0.000	0.000	0.001	375.169	0.002	0.001
MEA		0.000	496.768	0.000	0.000	0.000	0.000	0.000	0.000	496.768	0.000	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.004	0.000	0.002	0.004
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.001	0.002
METHANOL		0.000	0.000	0.000	0.000	0.000	0.000	0.000	18.266	0.000	25.827	26.069
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	3.304	3.762	0.440	0.542	0.509	0.076	0.000	0.091	0.093
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	3.266	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.412	0.000	5.492	5.268
ETLNCARB		0.000	0.000	0.000	0.000	0.087	6.438	0.000	0.066	0.000	1.802	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B1** Stream table of dimethyl carbonate from CCU process without allocation (cont'd)

Stream Name		S42	S43	S44	S45	S46	S47	S48	S49	S5	S50	S51
Stream Description												
Stream Phase		Liquid	Vapor	Vapor	Liquid	Vapor	Mixed	Vapor	Vapor	Liquid	Mixed	Mixed
Temperature	K	525.9367709	491.2724864	247.627264	397.85772	369.00227	369.00227	436.58756	436.587556	319.15	420	486.0321
Pressure	bar	10	125	9	20	1.21	1.21	10	19	1.013	11	2
Total Molecular Weight		69.76049402	44.01037942	44.0103794	35.9827335	44.0098	18.380164	33.080098	33.0800979	30.47995	25.069	69.76049
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.000	0.000	0.000	0.000	0.009	0.000	0.000	0.000	0.000	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.000	0.000	33.805	0.000	0.000	0.000	0.109	0.109	0.000	0.046	0.000
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.002	0.000	0.000	0.000	0.000	0.016	0.000	0.000	0.000	9.110	0.001
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.003	0.000	0.001	0.000
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.001	0.000
METHANOL		0.024	0.000	0.000	0.000	0.000	0.000	16.936	16.936	0.000	12.958	0.003
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.458	0.000	0.000	0.000	0.060	0.060	0.000	0.000	0.000
EG		3.267	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.758
DMCARB		0.277	0.000	0.000	0.000	0.000	0.000	0.804	0.804	0.000	0.000	0.029
ETLNCARB		1.803	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.631
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000



**Table B1** Stream table of dimethyl carbonate from CCU process without allocation (cont'd)

<b>Stream Name</b>		<b>S53</b>	<b>S54</b>	<b>S55</b>	<b>S56</b>	<b>S57</b>	<b>S58</b>	<b>S59</b>	<b>S6</b>	<b>S60</b>	<b>S7</b>	<b>S8</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Liquid</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Vapor</b>
Temperature	K	496.6336976	298.8707211	477.890527	523.15	262.18174	523.15	497.85576	319.150951	412.5431	319.15	1188.2
Pressure	bar	2	30	30	30	24.5	30	30	1.013	125	1.013	24
Total Molecular Weight		69.43373773	18.01527977	58.0797981	58.0797981	44.009795	58.079836	69.433738	30.4870441	44.00979	30.487	15.77359
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.038
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.000	0.000	0.000	0.000	0.000	0.881	0.000	34.722	0.780	34.722	10.656
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.000	0.000	0.000	0.364	0.000	0.004	0.000	374.938	0.000	374.938	8.898
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	496.871	0.000	496.871	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	24.744
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.756
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.204
METHANOL		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EG		3.169	0.000	0.000	3.169	0.000	4.411	3.169	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		1.780	0.000	0.000	1.780	0.000	0.018	1.780	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B1** Stream table of dimethyl carbonate from CCU process without allocation (cont'd)

Stream Name		S81	S82	S9	S91	S92	WASTE	WASTEWATER1	WATER	WATER_2
Stream Description										
Stream Phase		Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	K	319.15	319.15	372.791271	320	320	355.02924	438.3723227	298	298
Pressure	bar	1.013	1.013	1	1.013	1.013	1	11	1	1
Total Molecular Weight		61.08372116	61.08372116	18.0152798	32.2533298	18.01528	73.82612	20.30231458	18.0152798	18.01527977
<b>Total Weight Comp. Rates</b>	kg/s									
N2		0.000	0.000	0.000	0.000	0.000	0.000	7.76439E-16	0.000	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	1.45105E-22	0.000	0.000
CO2		0.000	0.000	0.000	0.000	0.000	1.475E-14	3.39184E-08	0.000	0.000
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.000	0.000	12.611	18.01528	18015.28	0.0013288	9.971361024	12.610696	0.363908656
MEA		0.142	61079.858	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	3.15935E-12	0.000	0.000
H2		0.000	0.000	0.000	0.000	0.000	0.000	5.70938E-15	0.000	0.000
METHANE		0.000	0.000	0.000	0.000	0.000	5.893E-19	6.46307E-12	0.000	0.000
METHANOL		0.000	0.000	0.000	0.000	0.000	0.0237644	3.454948128	0.000	0.000
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.000	1.397E-06	8.45107E-13	0.000	0.000
EG		0.000	0.000	0.000	0.000	0.000	0.0980128	9.49386E-13	0.000	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.2772495	4.04262E-10	0.000	0.000
ETLNCARB		0.000	0.000	0.000	0.000	0.000	0.0225809	2.46527E-13	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	6.284E-10	1.69713E-12	0.000	0.000

**Table B2** Equipment table of dimethyl carbonate from CCU process without allocation

<b>Pump</b>				
<b>Pump Name</b>		<b>P1</b>	<b>P2</b>	<b>P3</b>
Work	kW	61.30	1.33	17.22

<b>Compressor</b>					
<b>Compressor Name</b>		<b>C2</b>	<b>COMP_CH4</b>	<b>COMP_CO2</b>	<b>COMP_CO2_2</b>
Work	kW	83.45	9979.32	8148.79	4012.84

<b>Compressor (cont'd)</b>					
<b>Compressor Name</b>		<b>COMP_EO</b>	<b>COMP_H2O</b>	<b>COMP_MEOH</b>	<b>COMP_REC</b>
Work	kW	1477.86	12955.85	30792.90	6616.14

<b>Reactor</b>						
<b>ConReactor Name</b>		<b>DMCECSYN</b>	<b>ECSYN</b>	<b>EGSYN</b>	<b>MEOHSYN</b>	<b>COMREF</b>
Temperature	K	405.26	383.15	523.15	513.15	298.15
Pressure	bar	10	125	30	60	25
Duty	kJ/s	0	-7817.44	313.86	0.00	137960.10
Heat Of Reaction	kJ/s	-992.86	-1716.23	-249.70	-17447.57	49839.24
Product Enthalpy	kJ/s	5204.21	4698.34	1451.30	52950.45	48135.43
Feed Enthalpy	kJ/s	4924.51	5304.57	1317.16	27071.85	50577.34

**Table B2** Equipment table of dimethyl carbonate from CCU process without allocation (cont'd)

<b>Flash</b>		
<b>Flash Name</b>		<b>F1</b>
Temperature	K	333.15
Pressure	bar	59
DP	bar	0
Duty	kJ/s	1.08E-05

<b>Stream Calculator</b>		
<b>Stream Calculator Name</b>		<b>H2OREMOVAL</b>
Duty	kJ/s	0.000910
Overhead Product Temperature	K	369.00
Bottoms Product Temperature	K	369.00

<b>Heat Exchanger</b>						
<b>Hx Name</b>		<b>COOL_1</b>	<b>COOL_2</b>	<b>COOL_3</b>	<b>COOL_5</b>	<b>HEAT_1</b>
Duty	kJ/s	42335.32	103878.73	11797.76	18833.64	1606.03

<b>Heat Exchanger (cont'd)</b>					
<b>Hx Name</b>		<b>HEAT_2</b>	<b>HEAT_H2O</b>	<b>HX-1</b>	<b>HX-2</b>
Duty	kJ/s	713.17	32612.54	129674.39	243573.39

**Table B2** Equipment table of dimethyl carbonate from CCU process without allocation (cont'd)

<b>Column</b>		<b>DIST_DMC_1</b>	<b>DIST_DMC_2</b>	<b>DIST_DMC_3</b>	<b>DIST_EC_1</b>	<b>DIST_EG</b>
<b>Column Name</b>						
Condenser Duty	kJ/s	-106519.43	-64932.61	-1149.33	-61061.17	-1437.25
Reboiler Duty	kJ/s	106829.57	90786.26	572.17	63104.38	2143.34

<b>Column (cont'd)</b>		<b>DIST_MEOH_1</b>	<b>DIST_MEOH_2</b>	<b>T1</b>	<b>T2</b>
<b>Column Name</b>					
Condenser Duty	kJ/s	-5107.24	-50399.62	0.00	-534000.66
Reboiler Duty	kJ/s	0.00	50901.98	0.00	646937.18

**Table B3** Stream table of dimethyl carbonate from CCU process with allocation

<b>Stream Name</b>		<b>CO2</b>	<b>CO2PURGE</b>	<b>CO2_2</b>	<b>DMC</b>	<b>EC</b>	<b>EG</b>	<b>EO</b>	<b>MEOH</b>	<b>PURGE</b>	<b>PURGE2</b>	<b>PURGE3</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>
Temperature	K	312.712	312.712	312.712	492.876	614.284	595.478	298.150	403.482	333.150	389.593	247.627
Pressure	bar	1.21	1.21	1.21	20	10	25	1	10	59	10.5	9
Total Molecular Weight		42.4244	42.4244	42.4244	89.4847	87.6227	61.9399	44.0532	32.0755	22.4773	33.6347	44.0104
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.038	0.008	0.009	0.000	0.000	0.000	0.000	0.000	0.038	0.000	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		24.773	5.168	6.193	0.000	0.000	0.014	0.000	0.000	6.952	0.744	3.756
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.644	0.134	0.161	0.001	0.000	0.004	0.000	0.000	0.046	0.066	0.000
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	11.647	0.111	0.000
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.487	0.002	0.000
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.166	0.037	0.000
METHANOL		0.000	0.000	0.000	0.013	0.000	0.000	0.000	0.000	0.367	0.615	0.000
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.033	0.000	1.577	0.000	0.000	0.000	0.051
EG		0.000	0.000	0.000	0.000	0.000	4.411	0.000	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	4.031	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		0.000	0.000	0.000	0.000	6.438	0.018	0.000	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B3** Stream table of dimethyl carbonate from CCU process with allocation (cont'd)

<b>Stream Name</b>		<b>PURGEMEOH</b>	<b>PURGE_CO2_2</b>	<b>REC_CO2</b>	<b>REC_MEOH</b>	<b>S01</b>	<b>S01_R1</b>	<b>S01_R2</b>	<b>S02</b>	<b>S03</b>	<b>S1</b>	<b>S10</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Vapor</b>
Temperature	K	436.588	262.182	262.182	436.588	320.493	320.493	320.493	319.150	320.000	417.006	1174.81
Pressure	bar	19	24.5	24.5	19	1.567	1.567	1.567	1.013	1.013	10.5	25
Total Molecular Weight		33.0801	44.0098	44.0098	33.0801	29.8350	29.8350	29.8350	61.0837	18.0153	24.6880	24.6476
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.000	0.000	0.000	113.399	113.399	113.399	0.000	0.000	0.000	0.038
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.059	0.087	0.780	0.168	36.137	36.137	36.137	0.000	0.000	0.059	24.773
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.000	0.000	0.000	0.000	6.501	6.501	6.501	0.000	18015.28	9.974	13.255
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	61080.00	0.000	0.000	0.000
CO		0.001	0.000	0.000	0.004	0.000	0.000	0.000	0.000	0.000	0.001	0.000
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METHANE		0.001	0.000	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.001	11.230
METHANOL		9.120	0.000	0.000	26.056	0.000	0.000	0.000	0.000	0.000	15.984	0.000
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.033	0.000	0.000	0.093	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DMCARB		0.433	0.000	0.000	1.237	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B3** Stream table of dimethyl carbonate from CCU process with allocation (cont'd)

<b>Stream Name</b>		<b>S11</b>	<b>S12</b>	<b>S13</b>	<b>S14</b>	<b>S15</b>	<b>S16</b>	<b>S17</b>	<b>S18</b>	<b>S19</b>	<b>S2</b>	<b>S20</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Vapor</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Vapor</b>
Temperature	K	620.844	342.277	631.631	885.990	699.235	1188.200	729.235	756.342	513.150	384.000	816.059
Pressure	bar	25	1.58	25	25	25	25	24	60	60	1.58	59
Total Molecular Weight		16.0428	30.8203	42.4244	18.0153	24.6476	24.6479	15.7736	18.2175	18.2175	30.8203	23.2164
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.055	0.038	0.000	0.038	0.000	0.000	0.108	0.108	0.055	0.108
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.000	70.852	24.773	0.000	24.773	0.000	0.000	23.566	23.566	70.852	20.665
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.000	376.123	0.644	0.000	13.255	0.000	0.000	8.983	8.983	376.123	10.170
MEA		0.000	496.729	0.000	0.000	0.000	0.000	0.000	0.000	0.000	496.729	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	46.373	46.373	0.000	33.389
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	3.659	3.659	0.000	1.392
METHANE		11.230	0.000	0.000	0.000	11.230	0.000	0.000	6.226	6.226	0.000	6.226
METHANOL		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.681	0.681	0.000	17.647
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000



**Table B3** Stream table of dimethyl carbonate from CCU process with allocation (cont'd)

<b>Stream Name</b>		<b>S21</b>	<b>S22</b>	<b>S23</b>	<b>S24</b>	<b>S25</b>	<b>S26</b>	<b>S27</b>	<b>S28</b>	<b>S29</b>	<b>S3</b>	<b>S30</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Liquid</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Mixed</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Liquid</b>
Temperature	K	333.150	333.150	961.258	333.569	333.150	579.951	566.809	333.150	733.602	318.578	405.264
Pressure	bar	59	59	125	11	59	24	125	59	59	1.01	10
Total Molecular Weight		25.0688	22.4773	44.0098	25.0688	23.2164	18.2175	44.0135	22.4773	23.2164	27.3525	36.6843
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.108	0.000	0.000	0.108	0.108	0.000	0.070	0.108	113.343	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.803	19.862	6.193	0.803	20.665	23.566	40.778	12.910	20.665	0.006	0.168
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		10.040	0.130	0.000	10.040	10.170	8.983	0.000	0.085	10.170	5.316	0.002
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.142	0.000
CO		0.113	33.276	0.000	0.113	33.389	46.373	0.000	21.629	33.389	0.000	0.004
H2		0.002	1.390	0.000	0.002	1.392	3.659	0.000	0.904	1.392	0.000	0.000
METHANE		0.038	6.188	0.000	0.038	6.226	6.226	0.000	4.022	6.226	0.000	0.002
METHANOL		16.599	1.047	0.000	16.599	17.647	0.681	0.000	0.681	17.647	0.000	29.466
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.000	0.000	3.762	0.000	0.000	0.000	0.093
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.804
ETLNCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	6.438
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B3** Stream table of dimethyl carbonate from CCU process with allocation (cont'd)

<b>Stream Name</b>		<b>S31</b>	<b>S32</b>	<b>S34</b>	<b>S35</b>	<b>S36</b>	<b>S37</b>	<b>S38</b>	<b>S39</b>	<b>S4</b>	<b>S40</b>	<b>S41</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Vapor</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Mixed</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Liquid</b>	<b>Mixed</b>	<b>Liquid</b>
Temperature	K	312.722	399.504	640.788	383.150	383.150	320.945	247.627	417.541	319.150	408.315	397.245
Pressure	bar	1.21	1.778	125	125	125	10	9	10	1.778	10	9
Total Molecular Weight		42.4235	30.4799	44.0532	44.0135	47.4406	47.4406	44.0104	36.6843	30.4799	38.7055	35.9827
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.055	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		36.135	34.722	0.000	40.778	36.471	37.561	37.561	0.165	34.722	0.125	0.168
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.940	375.169	0.000	0.000	0.000	0.000	0.000	0.001	375.169	0.002	0.001
MEA		0.000	496.768	0.000	0.000	0.000	0.000	0.000	0.000	496.768	0.000	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.004	0.000	0.002	0.004
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.001	0.002
METHANOL		0.000	0.000	0.000	0.000	0.000	0.000	0.000	18.266	0.000	25.827	26.069
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	3.304	3.762	0.440	0.542	0.509	0.076	0.000	0.091	0.093
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	3.266	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.412	0.000	5.492	5.268
ETLNCARB		0.000	0.000	0.000	0.000	0.087	6.438	0.000	0.066	0.000	1.802	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B3** Stream table of dimethyl carbonate from CCU process with allocation (cont'd)

<b>Stream Name</b>		<b>S42</b>	<b>S43</b>	<b>S44</b>	<b>S45</b>	<b>S46</b>	<b>S47</b>	<b>S48</b>	<b>S49</b>	<b>S5</b>	<b>S50</b>	<b>S51</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Liquid</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Mixed</b>	<b>Mixed</b>
Temperature	K	525.937	491.272	247.627	397.858	369.002	369.002	436.588	436.588	319.150	420.000	486.032
Pressure	bar	10	125	9	20	1.21	1.21	10	19	1.013	11	2
Total Molecular Weight		69.7605	44.0104	44.0104	35.9827	44.0098	18.3802	33.0801	33.0801	30.4799	25.0688	69.7605
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.000	0.000	0.000	0.000	0.009	0.000	0.000	0.000	0.000	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.000	0.000	33.805	0.000	0.000	0.000	0.109	0.109	0.000	0.046	0.000
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.002	0.000	0.000	0.000	0.000	0.016	0.000	0.000	0.000	9.110	0.001
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.003	0.000	0.001	0.000
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.001	0.000
METHANOL		0.024	0.000	0.000	0.000	0.000	0.000	16.936	16.936	0.000	12.958	0.003
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.458	0.000	0.000	0.000	0.060	0.060	0.000	0.000	0.000
EG		3.267	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.758
DMCARB		0.277	0.000	0.000	0.000	0.000	0.000	0.804	0.804	0.000	0.000	0.029
ETLNCARB		1.803	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.631
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B3** Stream table of dimethyl carbonate from CCU process with allocation (cont'd)

<b>Stream Name</b>		<b>S53</b>	<b>S54</b>	<b>S55</b>	<b>S56</b>	<b>S57</b>	<b>S58</b>	<b>S59</b>	<b>S6</b>	<b>S60</b>	<b>S7</b>	<b>S8</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Liquid</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Vapor</b>
Temperature	K	496.634	298.871	477.891	523.150	262.182	523.150	497.856	319.151	412.543	319.151	1188.200
Pressure	bar	2	30	30	30	24.5	30	30	1.013	125	1.013	24
Total Molecular Weight		69.4337	18.0153	58.0798	58.0798	44.0098	58.0798	69.4337	30.4870	44.0098	30.4870	15.7736
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.038
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.000	0.000	0.000	0.000	0.000	0.881	0.000	34.722	0.780	34.722	10.656
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.000	0.000	0.000	0.364	0.000	0.004	0.000	374.938	0.000	374.938	8.898
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	496.871	0.000	496.871	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	24.744
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.756
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.204
METHANOL		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EG		3.169	0.000	0.000	3.169	0.000	4.411	3.169	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		1.780	0.000	0.000	1.780	0.000	0.018	1.780	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B3** Stream table of dimethyl carbonate from CCU process with allocation (cont'd)

Stream Name		S81	S82	S9	S91	S92	WASTE	WASTEWATER1	WATER	WATER_2
Stream Description										
Stream Phase		Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	K	319.150	319.150	372.791	320.000	320.000	355.029	438.372	298.000	298.000
Pressure	bar	1.013	1.013	1	1.013	1.013	1	11	1	1
Total Molecular Weight		61.0837	61.0837	18.0153	32.2533	18.0153	73.8261	20.3023	18.0153	18.0153
<b>Total Weight Comp. Rates</b>	kg/s									
N2		0.000	0.000	0.000	0	0	0	7.76439E-16	0	0
O2		0.000	0.000	0.000	0	0	0	1.45105E-22	0	0
CO2		0.000	0.000	0.000	0	0	1.5E-14	3.39184E-08	0	0
SO2		0.000	0.000	0.000	0	0	0	0	0	0
H2O		0.000	0.000	12.611	18.01528	18015.3	0.00133	9.971361024	12.6107	0.363909
MEA		0.142	61079.858	0.000	0	0	0	0	0	0
CO		0.000	0.000	0.000	0	0	0	3.15935E-12	0	0
H2		0.000	0.000	0.000	0	0	0	5.70938E-15	0	0
METHANE		0.000	0.000	0.000	0	0	5.9E-19	6.46307E-12	0	0
METHANOL		0.000	0.000	0.000	0	0	0.02376	3.454948128	0	0
DME		0.000	0.000	0.000	0	0	0	0	0	0
EO		0.000	0.000	0.000	0	0	1.4E-06	8.45107E-13	0	0
EG		0.000	0.000	0.000	0	0	0.09801	9.49386E-13	0	0
DMCARB		0.000	0.000	0.000	0	0	0.27725	4.04262E-10	0	0
ETLNCARB		0.000	0.000	0.000	0	0	0.02258	2.46527E-13	0	0
TOLUENE		0.000	0.000	0.000	0	0	6.3E-10	1.69713E-12	0	0

**Table B4** Equipment table of dimethyl carbonate from CCU process with allocation

<b>Pump</b>				
<b>Pump Name</b>		<b>P1</b>	<b>P2</b>	<b>P3</b>
Work	kW	23.68	0.51	6.65

<b>Compressor</b>					
<b>Compressor Name</b>		<b>C2</b>	<b>COMP_CH4</b>	<b>COMP_CO2</b>	<b>COMP_CO2_2</b>
Work	kW	32.24	3855.75	3148.48	1550.46

<b>Compressor (cont'd)</b>					
<b>Compressor Name</b>		<b>COMP_EO</b>	<b>COMP_H2O</b>	<b>COMP_MEOH</b>	<b>COMP_REC</b>
Work	kW	571.01	5005.81	11897.58	2556.31

<b>Reactor</b>						
<b>ConReactor Name</b>		<b>DMCECSYN</b>	<b>ECSYN</b>	<b>EGSYN</b>	<b>MEOHSYN</b>	<b>COMREF</b>
Temperature	K	405.26	383.15	523.15	513.15	298.15
Pressure	bar	10	125	30	60	25
Duty	kJ/s	0	-3020.46	121.27	0.00	53304.20
Heat Of Reaction	kJ/s	-992.86	-1716.23	-249.70	-17447.57	49839.24
Product Enthalpy	kJ/s	5204.21	4698.34	1451.30	52950.45	48135.43
Feed Enthalpy	kJ/s	4924.51	5304.57	1317.16	27071.85	50577.34

**Table B4** Equipment table of dimethyl carbonate from CCU process with allocation (cont'd)

<b>Flash</b>		
<b>Flash Name</b>		<b>F1</b>
Temperature	K	333.15
Pressure	bar	59
DP	bar	0
Duty	kJ/s	4.16E-06

<b>Stream Calculator</b>		
<b>Stream Calculator Name</b>		<b>H2OREMOVAL</b>
Duty	kJ/s	0.000352
Overhead Product Temperature	K	369.00
Bottoms Product Temperature	K	369.00

<b>Heat Exchanger</b>						
<b>Hx Name</b>		<b>COOL_1</b>	<b>COOL_2</b>	<b>COOL_3</b>	<b>COOL_5</b>	<b>HEAT_1</b>
Duty	kJ/s	-16357.27	-40136.05	-4558.35	-7276.83	620.53

<b>Heat Exchanger (cont'd)</b>					
<b>Hx Name</b>		<b>HEAT_2</b>	<b>HEAT_H2O</b>	<b>HX-1</b>	<b>HX-2</b>
Duty	kJ/s	275.55	12600.64	50102.82	-94110.44

**Table B4** Equipment table of dimethyl carbonate from CCU process with allocation (cont'd)

<b>Column</b>						
<b>Column Name</b>		<b>DIST_DMC_1</b>	<b>DIST_DMC_2</b>	<b>DIST_DMC_3</b>	<b>DIST_EC_1</b>	<b>DIST_EG</b>
Condenser Duty	kJ/s	-41156.35	-25088.28	-444.07	-23592.45	-555.32
Reboiler Duty	kJ/s	41276.18	35077.46	221.07	24381.90	828.13

<b>Column (cont'd)</b>					
<b>Column Name</b>		<b>DIST_MEOH_1</b>	<b>DIST_MEOH_2</b>	<b>T1</b>	<b>T2</b>
Condenser Duty	kJ/s	-1973.30	-19473.11	0.00	-206324.01
Reboiler Duty	kJ/s	0.00	19667.20	0.00	249959.75



**Table B5** Stream table of ethylene glycol (co product) from CCU process with allocation

<b>Stream Name</b>		<b>CO2</b>	<b>CO2PURGE</b>	<b>CO2_2</b>	<b>DMC</b>	<b>EC</b>	<b>EG</b>	<b>EO</b>	<b>MEOH</b>	<b>PURGE</b>	<b>PURGE2</b>	<b>PURGE3</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>
Temperature	K	312.71	312.71	312.71	492.88	614.28	595.48	298.15	403.48	333.15	389.59	247.63
Pressure	bar	1.21	1.21	1.21	20	10	25	1	10	59	10.5	9
Total Molecular Weight		42.42437	42.4243711	42.42437	89.48468	87.6227	61.93991	44.05316	32.07548	22.47725	33.63472	44.01038
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.038	0.008	0.009	0.000	0.000	0.000	0.000	0.000	0.038	0.000	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		24.773	5.168	6.193	0.000	0.000	0.014	0.000	0.000	6.952	0.744	3.756
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.644	0.134	0.161	0.001	0.000	0.004	0.000	0.000	0.046	0.066	0.000
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	11.647	0.111	0.000
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.487	0.002	0.000
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.166	0.037	0.000
METHANOL		0.000	0.000	0.000	0.013	0.000	0.000	0.000	0.000	0.367	0.615	0.000
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.033	0.000	1.726	0.000	0.000	0.000	0.051
EG		0.000	0.000	0.000	0.000	0.000	4.411	0.000	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	4.031	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		0.000	0.000	0.000	0.000	6.438	0.018	0.000	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B5** Stream table of ethylene glycol (co product) from CCU process with allocation (cont'd)

Stream Name		PURGEMEOH	PURGE_CO2_2	REC_CO2	REC_MEOH	S01	S01_R1	S01_R2	S02	S03	S1	S10
Stream Description												
Stream Phase		Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor	Liquid	Liquid	Liquid	Vapor
Temperature	K	436.59	262.18	262.18	436.59	320.49	320.49	320.49	319.15	320.00	417.01	1174.81
Pressure	bar	19	24.5	24.5	19	1.567	1.567	1.567	1.013	1.013	10.5	25
Total Molecular Weight		33.0800979	44.00979474	44.00979	33.0800979	29.835	29.835	29.835	61.08372	18.01528	24.68799	24.6476
Total Weight Comp. Rates	kg/s											
N2		0.000	0.000	0.000	0.000	113.399	113.399	113.399	0.000	0.000	0.000	0.038
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.059	0.087	0.780	0.168	36.137	36.137	36.137	0.000	0.000	0.059	24.773
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.000	0.000	0.000	0.000	6.501	6.501	6.501	0.000	18015.28	9.974	13.255
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	61080.00	0.000	0.000	0.000
CO		0.001	0.000	0.000	0.004	0.000	0.000	0.000	0.000	0.000	0.001	0.000
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METHANE		0.001	0.000	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.001	11.230
METHANOL		9.120	0.000	0.000	26.056	0.000	0.000	0.000	0.000	0.000	15.984	0.000
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.033	0.000	0.000	0.093	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DMCARB		0.433	0.000	0.000	1.237	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B5** Stream table of ethylene glycol (co product) from CCU process with allocation (cont'd)

<b>Stream Name</b>		<b>S11</b>	<b>S12</b>	<b>S13</b>	<b>S14</b>	<b>S15</b>	<b>S16</b>	<b>S17</b>	<b>S18</b>	<b>S19</b>	<b>S2</b>	<b>S20</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Vapor</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Vapor</b>
Temperature	K	620.84	342.28	631.63	885.99	699.23	1188.20	729.23	756.34	513.15	384.00	816.06
Pressure	bar	25	1.58	25	25	25	25	24	60	60	1.58	59
Total Molecular Weight		16.0427609	30.8203054	42.42437	18.0152798	24.6476	24.6479	15.7736	18.21748	18.21748	30.82031	23.2164
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.055	0.038	0.000	0.038	0.000	0.000	0.108	0.108	0.055	0.108
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.000	70.852	24.773	0.000	24.773	0.000	0.000	23.566	23.566	70.852	20.665
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.000	376.123	0.644	0.000	13.255	0.000	0.000	8.983	8.983	376.123	10.170
MEA		0.000	496.729	0.000	0.000	0.000	0.000	0.000	0.000	0.000	496.729	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	46.373	46.373	0.000	33.389
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	3.659	3.659	0.000	1.392
METHANE		11.230	0.000	0.000	0.000	11.230	0.000	0.000	6.226	6.226	0.000	6.226
METHANOL		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.681	0.681	0.000	17.647
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B5** Stream table of ethylene glycol (co product) from CCU process with allocation (cont'd)

<b>Stream Name</b>		<b>S21</b>	<b>S22</b>	<b>S23</b>	<b>S24</b>	<b>S25</b>	<b>S26</b>	<b>S27</b>	<b>S28</b>	<b>S29</b>	<b>S3</b>	<b>S30</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Liquid</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Mixed</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Liquid</b>
Temperature	K	333.15	333.15	961.26	333.57	333.15	579.95	566.81	333.15	733.60	318.58	405.26
Pressure	bar	59	59	125	11	59	24	125	59	59	1.01	10
Total Molecular Weight		25.0687587	22.47725322	44.0098	25.0687587	23.2164	18.2175	44.0135	22.47725	23.21641	27.35249	36.6843
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.108	0.000	0.000	0.108	0.108	0.000	0.070	0.108	113.343	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.803	19.862	6.193	0.803	20.665	23.566	40.778	12.910	20.665	0.006	0.168
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		10.040	0.130	0.000	10.040	10.170	8.983	0.000	0.085	10.170	5.316	0.002
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.142	0.000
CO		0.113	33.276	0.000	0.113	33.389	46.373	0.000	21.629	33.389	0.000	0.004
H2		0.002	1.390	0.000	0.002	1.392	3.659	0.000	0.904	1.392	0.000	0.000
METHANE		0.038	6.188	0.000	0.038	6.226	6.226	0.000	4.022	6.226	0.000	0.002
METHANOL		16.599	1.047	0.000	16.599	17.647	0.681	0.000	0.681	17.647	0.000	29.466
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.000	0.000	3.762	0.000	0.000	0.000	0.093
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.804
ETLNCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	6.438
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B5** Stream table of ethylene glycol (co product) from CCU process with allocation (cont'd)

<b>Stream Name</b>		<b>S31</b>	<b>S32</b>	<b>S34</b>	<b>S35</b>	<b>S36</b>	<b>S37</b>	<b>S38</b>	<b>S39</b>	<b>S4</b>	<b>S40</b>	<b>S41</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Vapor</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Mixed</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Liquid</b>	<b>Mixed</b>	<b>Liquid</b>
Temperature	K	312.72	399.50	640.79	383.15	383.15	320.94	247.63	417.54	319.15	408.31	397.24
Pressure	bar	1.21	1.778	125	125	125	10	9	10	1.778	10	9
Total Molecular Weight		42.4235313	30.47994507	44.05316	44.0134593	47.4406	47.4406	44.0104	36.6843	30.47995	38.70548	35.9827
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.055	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		36.135	34.722	0.000	40.778	36.471	37.561	37.561	0.165	34.722	0.125	0.168
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.940	375.169	0.000	0.000	0.000	0.000	0.000	0.001	375.169	0.002	0.001
MEA		0.000	496.768	0.000	0.000	0.000	0.000	0.000	0.000	496.768	0.000	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.004	0.000	0.002	0.004
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.001	0.002
METHANOL		0.000	0.000	0.000	0.000	0.000	0.000	0.000	18.266	0.000	25.827	26.069
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	3.304	3.762	0.440	0.542	0.509	0.076	0.000	0.091	0.093
EG		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	3.266	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.412	0.000	5.492	5.268
ETLNCARB		0.000	0.000	0.000	0.000	0.087	6.438	0.000	0.066	0.000	1.802	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B5** Stream table of ethylene glycol (co product) from CCU process with allocation (cont'd)

<b>Stream Name</b>		<b>S42</b>	<b>S43</b>	<b>S44</b>	<b>S45</b>	<b>S46</b>	<b>S47</b>	<b>S48</b>	<b>S49</b>	<b>S5</b>	<b>S50</b>	<b>S51</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Liquid</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Vapor</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Mixed</b>	<b>Mixed</b>
Temperature	K	525.94	491.27	247.63	397.86	369.00	369.00	436.59	436.59	319.15	420.00	486.03
Pressure	bar	10	125	9	20	1.21	1.21	10	19	1.013	11	2
Total Molecular Weight		69.760494	44.01037942	44.01038	35.9827335	44.0098	18.3802	33.0801	33.0801	30.47995	25.06876	69.7605
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.000	0.000	0.000	0.000	0.009	0.000	0.000	0.000	0.000	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.000	0.000	33.805	0.000	0.000	0.000	0.109	0.109	0.000	0.046	0.000
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.002	0.000	0.000	0.000	0.000	0.016	0.000	0.000	0.000	9.110	0.001
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.003	0.000	0.001	0.000
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.001	0.000
METHANOL		0.024	0.000	0.000	0.000	0.000	0.000	16.936	16.936	0.000	12.958	0.003
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.458	0.000	0.000	0.000	0.060	0.060	0.000	0.000	0.000
EG		3.267	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.758
DMCARB		0.277	0.000	0.000	0.000	0.000	0.000	0.804	0.804	0.000	0.000	0.029
ETLNCARB		1.803	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.631
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B5** Stream table of ethylene glycol (co product) from CCU process with allocation (cont'd)

<b>Stream Name</b>		<b>S53</b>	<b>S54</b>	<b>S55</b>	<b>S56</b>	<b>S57</b>	<b>S58</b>	<b>S59</b>	<b>S6</b>	<b>S60</b>	<b>S7</b>	<b>S8</b>
<b>Stream Description</b>												
<b>Stream Phase</b>		<b>Liquid</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Mixed</b>	<b>Liquid</b>	<b>Liquid</b>	<b>Vapor</b>	<b>Liquid</b>	<b>Vapor</b>
Temperature	K	496.63	298.87	477.89	523.15	262.18	523.15	497.86	319.15	412.54	319.15	1188.20
Pressure	bar	2	30	30	30	24.5	30	30	1.013	125	1.013	24
Total Molecular Weight		69.4337377	18.01527977	58.0798	58.0797981	44.0098	58.0798	69.4337	30.48704	44.00979	30.48704	15.7736
<b>Total Weight Comp. Rates</b>	kg/s											
N2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.038
O2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO2		0.000	0.000	0.000	0.000	0.000	0.881	0.000	34.722	0.780	34.722	10.656
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.000	0.000	0.000	0.364	0.000	0.004	0.000	374.938	0.000	374.938	8.898
MEA		0.000	0.000	0.000	0.000	0.000	0.000	0.000	496.871	0.000	496.871	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	24.744
H2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.756
METHANE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	2.204
METHANOL		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EG		3.169	0.000	0.000	3.169	0.000	4.411	3.169	0.000	0.000	0.000	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ETLNCARB		1.780	0.000	0.000	1.780	0.000	0.018	1.780	0.000	0.000	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**Table B5** Stream table of ethylene glycol (co product) from CCU process with allocation (cont'd)

Stream Name		S81	S82	S9	S91	S92	WASTE	WASTEWATER1	WATER	WATER_2
Stream Description										
Stream Phase		Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	K	319.15	319.15	372.79	320.00	320.00	355.03	438.37	298.00	298.00
Pressure	bar	1.013	1.013	1	1.013	1.013	1	11	1	1
Total Molecular Weight		61.0837212	61.08372116	18.01528	32.2533298	18.0153	73.8261	20.30231458	18.01528	18.01528
<b>Total Weight Comp. Rates</b>	kg/s									
N2		0.000	0.000	0.000	0.000	0.000	0.000	7.76439E-16	0.000	0.000
O2		0.000	0.000	0.000	0.000	0.000	0.000	1.45105E-22	0.000	0.000
CO2		0.000	0.000	0.000	0.000	0.000	1.5E-14	3.39184E-08	0.000	0.000
SO2		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H2O		0.000	0.000	12.611	18.01528	18015.3	0.00133	9.971361024	12.6107	0.363909
MEA		0.142	61079.858	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CO		0.000	0.000	0.000	0.000	0.000	0.000	3.15935E-12	0.000	0.000
H2		0.000	0.000	0.000	0.000	0.000	0.000	5.70938E-15	0.000	0.000
METHANE		0.000	0.000	0.000	0.000	0.000	5.9E-19	6.46307E-12	0.000	0.000
METHANOL		0.000	0.000	0.000	0.000	0.000	0.02376	3.454948128	0.000	0.000
DME		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EO		0.000	0.000	0.000	0.000	0.000	1.4E-06	8.45107E-13	0.000	0.000
EG		0.000	0.000	0.000	0.000	0.000	0.09801	9.49386E-13	0.000	0.000
DMCARB		0.000	0.000	0.000	0.000	0.000	0.27725	4.04262E-10	0.000	0.000
ETLNCARB		0.000	0.000	0.000	0.000	0.000	0.02258	2.46527E-13	0.000	0.000
TOLUENE		0.000	0.000	0.000	0.000	0.000	6.3E-10	1.69713E-12	0.000	0.000



**Table B6** Equipment table of ethylene glycol (co product) from CCU process with allocation

<b>Pump</b>					
<b>Pump Name</b>		<b>P1</b>	<b>P2</b>	<b>P3</b>	
Work	kW	37.61	0.81	10.57	

<b>Compressor</b>					
<b>Compressor Name</b>		<b>C2</b>	<b>COMP_CH4</b>	<b>COMP_CO2</b>	<b>COMP_CO2_2</b>
Work	kW	51.20	6123.57	5000.31	2462.38

<b>Compressor (cont'd)</b>					
<b>Compressor Name</b>		<b>COMP_EO</b>	<b>COMP_H2O</b>	<b>COMP_MEOH</b>	<b>COMP_REC</b>
Work	kW	906.85	7950.05	18895.32	4059.84

<b>Reactor</b>						
<b>ConReactor Name</b>		<b>DMCECSYN</b>	<b>ECSYN</b>	<b>EGSYN</b>	<b>MEOHSYN</b>	<b>COMREF</b>
Temperature	K	405.26	383.15	523.15	513.15	298.15
Pressure	bar	10	125	30	60	25
Duty	kJ/s	0	-4796.98	192.59	0.00	84655.89
Heat Of Reaction	kJ/s	-1576.82	-2725.66	-396.57	-27709.63	79152.95
Product Enthalpy	kJ/s	8265.14	7461.75	2304.90	84094.07	76447.02
Feed Enthalpy	kJ/s	7820.93	8424.54	2091.86	42994.57	80325.18

**Table B6** Equipment table of ethylene glycol (co product) from CCU process with allocation (cont'd)

<b>Flash</b>		
<b>Flash Name</b>		<b>F1</b>
Temperature	K	333.15
Pressure	bar	59
DP	bar	0
Duty	kJ/s	6.61E-06

<b>Stream Calculator</b>		
<b>Stream Calculator Name</b>		<b>H2OREMOVAL</b>
Duty	kJ/s	0.000559
Overhead Product Temperature	K	369.00
Bottoms Product Temperature	K	369.00

<b>Heat Exchanger</b>						
<b>Hx Name</b>		<b>COOL_1</b>	<b>COOL_2</b>	<b>COOL_3</b>	<b>COOL_5</b>	<b>HEAT_1</b>
Duty	kJ/s	-25978.05	-63742.68	-7239.41	-11556.81	985.50

<b>Heat Exchanger (cont'd)</b>					
<b>Hx Name</b>		<b>HEAT_2</b>	<b>HEAT_H2O</b>	<b>HX-1</b>	<b>HX-2</b>
Duty	kJ/s	437.62	20011.90	79571.57	-149462.95

**Table B6** Equipment table of ethylene glycol (co product) from CCU process with allocation (cont'd)

<b>Column</b>						
<b>Column Name</b>		<b>DIST_DMC_1</b>	<b>DIST_DMC_2</b>	<b>DIST_DMC_3</b>	<b>DIST_EC_1</b>	<b>DIST_EG</b>
Condenser Duty	kJ/s	-65363.08	-39844.33	-705.26	-37468.71	-881.93
Reboiler Duty	kJ/s	65553.39	55708.80	351.10	38722.48	1315.21

<b>Column (cont'd)</b>					
<b>Column Name</b>		<b>DIST_MEOH_1</b>	<b>DIST_MEOH_2</b>	<b>T1</b>	<b>T2</b>
Condenser Duty	kJ/s	-3133.93	-30926.51	0.00	-327676.65
Reboiler Duty	kJ/s	0.00	31234.77	0.00	396977.43

## Appendix C Characterization Factors of Water Scarcity Footprint in Denmark

**Table C1** Characterization factors of water scarcity footprint in Denmark

Month	Agriculture	Non-Agriculture	Unknown
January	0.00000	2.02996	2.02996
February	0.00000	2.18195	2.18195
March	0.40049	2.03375	2.03307
April	0.48909	2.60806	2.57112
May	1.50996	3.65205	2.36868
June	2.45364	5.78095	2.81740
July	3.33053	7.72762	3.53000
August	4.23307	9.00941	4.59546
September	3.97819	8.81124	5.31507
October	2.99350	6.75027	6.49582
November	0.00000	4.69554	4.69554
December	0.00000	2.68438	2.68438

## Appendix D Ecological Footprint in each unit of Denmark

**Table D1** Ecological Footprint in each unit of Denmark

	<b>Biocapacity (gha)</b>	<b>Ecological Footprint (gha per person)</b>	<b>Ecological Footprint (gha)</b>	<b>Ecological Footprint (Number of Earths)</b>
<b>Built-up Land</b>	1291929.35610	0.22971	1291929.35610	0.13470
<b>Carbon</b>	0.00000	3.11296	17508215.39721	1.82547
<b>Cropland</b>	12311400.80860	1.13039	6357629.60700	0.66287
<b>Fishing Grounds</b>	10170337.75348	0.24145	1357972.67961	0.14159
<b>Forest Products</b>	1907354.39436	0.89322	5023717.20024	0.52379
<b>Grazing Land</b>	43690.96684	0.50065	2815810.45556	0.29359
<b>Total</b>	25724713.27937	6.10838	34355274.69571	3.58200

